Catalyst evaluation for oxygen reduction reaction in concentrated phosphoric acid at elevated temperatures

Phosphoric acid is the common electrolyte for high-temperature polymer electrolyte fuel cells (HT-PEMFCs) that have advantages such as enhanced CO tolerance and simplified heat and water management. The currently used rotating disk electrode technique is limited to tests in dilute solutions at low temperatures and hence is not suitable for catalyst evaluation for HT-PEMFCs. In this study, we have designed and constructed a half-cell setup to measure the intrinsic activities of catalysts towards the oxygen reduction reaction (ORR) in conditions close to HT-PEMFC cathodes. By optimization of the hydrophobic characteristics of electrodes and the catalyst layer thickness, ORR activities of typical Pt/C catalysts are successfully measured in concentrated phosphoric acid at temperatures above 100 °C. In terms of mass-specific activities, the catalyst exhibits about two times higher activity in the half-cell electrode than that observed in fuel cells, indicating the feasibility of the technique as well as the potential for further improvement of fuel cell electrode performance.
Effect of spherical porosity on co-fired dense/porous zirconia bi-layers cambering

Geometrical instability leading to cambering is recorded during co-sintering of zirconia dense/porous bi-layered planar structures. Sintering strain in the bi-layers rises mainly from mismatch between the different porosity volume fractions at the layers and their interface. In this paper, we analyze the model case of dense taped of 8 mol% Y$_2$O$_3$-stabilized ZrO$_2$ laminated on ca. 400 μ thick 3 mol% Y$_2$O$_3$ doped zirconia porous tapes, with homogenous spherical porosity of 13 vol%.
46 vol%, and 54 vol%. Sintering stress during densification is evaluated from the shrinkage rates and viscoelastic behavior during sintering by thermo-mechanical analysis, using cyclic loading dilatometry. The camber development of the bi-layers is measured by in-situ optical dilatometry. In accordance with the model prediction, cambering can be controlled tuning the porosity while achieving a synergetic effect between densification and formation of open porosity at the bilayers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Universidade Federal do ABC
Authors: Teocoli, F. (Intern), Marani, D. (Ekstern), Kiebach, W. (Intern), Esposito, V. (Intern)
Pages: 173-179
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: European Ceramic Society. Journal
Volume: 38
Issue number: 1
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.392 SNIP 1.945
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.381 SNIP 1.724
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.146 SNIP 1.645
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.22 SNIP 1.76
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.191 SNIP 1.67
Web of Science (2006): Indexed yes
High stability of benzotriazole and benzodithiophene containing medium band-gap polymer solar cell

The improvement of polymer solar cell stability is a challenge for the scientists and has significant implications commercially. In this study, we investigated the stability of a novel P-SBTBDT active material applied in an inverted type solar cell. Detailed stability experiments comprising shelf life, laboratory weathering and outdoor testing were carried out according to ISOS testing guidelines. Shelf life showed that P-SBTBDT solar cells were very stable after 840 h with encapsulation. Although accelerated weathering aging tests are a very harsh, the devices remained stable after the burn-in phase with T50 from 700 to 840 h, with some P-SBTBDT solar cells did not reach T50 in the time span of the test. Degradation tests on the P-SBTBDT solar cells which were carried out under natural solar light indicated that T40 was reached after 840 h. The results of dark, light, damp and dry stability tests showed that most of the degradation was provoked by failure of the encapsulation. The experiments indicated that P-SBTBDT solar cells are sensitive to light and oxygen but are strikingly stable under humid conditions. Further developments for minimizing the degradation effects using UV-filters and better encapsulation are some of the necessary improvements in further research.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Organic Energy Materials, Department of Energy Conversion and Storage, Middle East Technical University, Yildiz Technical University, TUBITAK
Pages: 433-444
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 174
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Mechanical stability of roll-to-roll printed solar cells under cyclic bending and torsion

The ability of printed organic solar cells (OSCs) to survive repeated mechanical deformation is critical to large-scale implementation. This paper reports an investigation into the mechanical stability of OSCs through bending and torsion testing of whole printed modules. Two types of modules are used that differ slightly in thickness as well as on the basis of the electrode materials: silver nanowires or carbon-based inks. Each type of module is subjected to two different mechanical modes of deformation, bending and torsion, of several thousand cycles per module using a purpose-built robotic device. Analysis of the distribution of stress in the devices performed by finite-element modeling predicts the locations of failure. Failure upon bending originates at the laser-cut edges of the modules from shear at the clamp/module interface leading to crazing of the plastic barrier encapsulant foils. This crazing leads to eventual delamination due first to decohesion of the active layer at the edge of the modules and later to deadhesion between the PEDOT:PSS (electrode) and P3HT:PCBM (semiconductor) layers. The torsion mode imposes greater stresses than the bending mode and thus leads to failure at fewer strain cycles. Failure during torsion occurs through crack propagation initiated at stress concentrations on the edges of the module that were imposed by their rectangular geometry and ultimately leads to bifurcation of the entire module. Rather than the differences in electrode materials, the differences in survivability between the two types of modules are attributed mostly to the thickness of the substrate materials used, with the thinner substrate used in the carbon-based modules (~160 Åm) failing at fewer strain cycles than the substrate used in the silver-nanowire-based modules (~190 Åm). Taken together, the results suggest ways in which the lifetimes of devices can be
extended by the layouts of modules and choices of materials.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of California
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Pages: 7-15
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Solar Energy Materials and Solar Cells
Volume: 174
ISSN (Print): 0927-0248
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.524 SNIP 2.121
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.991 SNIP 1.977
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.654 SNIP 1.458
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.359 SNIP 1.488
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.447 SNIP 1.799
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.141 SNIP 1.619
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.932 SNIP 1.178
Structural and superconducting characteristics of YBa$_2$Cu$_3$O$_{7-x}$ films grown by fluorine-free metal-organic deposition route

Microstructure and superconducting performance of YBa$_2$Cu$_3$O$_{7-y}$ (YBCO) films deposited on LaAlO$_3$ single crystal (LAO) substrates by a fluorine-free metal-organic deposition (FF-MOD) technique, have been studied by means of X-ray reciprocal space mapping (RSM), cross-sectional transmission electron microscopy (TEM) and magneto-optical (MO) imaging. Combining the X-ray diffraction and the TEM cross-sectional analysis, it is revealed that stacking faults, i.e. YBa$_2$Cu$_4$O$_x$ intergrowths, and ab-plane twins are main defects in the FF-MOD YBCO films. Due to the highly epitaxial growth mechanism related to transient liquid phase, the LAO twinned substrate structure is also inherited in the FF-YBCO films. The low-density planar defects containing dislocations parallel to c-axis result in stripy patterns observed in the MO images. For comparison, the low-fluorine (LF) MOD film show a texture mosaic spread in the ab plane and is little influenced by the LAO twinning underneath, implying the severe structural disorder most likely associated with the large amount of small-angle grain boundaries. Moreover, the higher density of stacking faults was also detected by XRD θ-2θ, scan in the LF-MOD film. It is suggested that associated partial dislocations formed at the boundary between the stacking faults and YBCO matrix act as strong linear (or dot) pinning centers. These structural characteristics are well in line with the better superconducting performance of the low fluorine-MOD film, in particular under external magnetic field at 77 K. This work offers an in-depth insight into the correlation between the microstructure and superconductivity in the MOD YBCO films.
Graphitic layer encapsulated iron based nanoparticles (G@FeNPs) have recently been disclosed as an interesting type of highly active electrocatalysts for the oxygen reduction reaction (ORR). However, the complex composition of the metal-containing components and their contributions in catalysis remain unclear. As a representative catalyst of the unique encapsulated structure, a series of G@FeNPs catalysts were prepared by a high-pressure pyrolytic process with uniform and essentially identical morphologies but varied compositions. The catalysts exhibited a high onset potential of 0.85 V at 0.1 mA cm$^{-2}$ in acidic media. By $^{57}$Fe-Mössbauer spectroscopy the iron containing components were identified including α-Fe, γ-Fe, γ-Fe$_2$O$_3$, and Fe$_3$C as well as a minor doublet component due to Fe$^{3+}$ in high spin and/or Fe$^{2+}$ in low spin state. The ORR activities are evaluated in terms of the mass specific kinetic current density found to be positively correlated with the Fe$_3$C content in the range of study, indicating involvement of the encapsulated nanoparticles in the ORR catalysis. The recognition of the Fe compositions and active sites provides new insights to the confined Fe-based ORR electrocatalysts and therefore options for further development of non-precious metal materials.
METHOD AND APPARATUS FOR CHARACTERIZATION OF A SOLAR CELL
The present disclosure relates to a method for characterization of a solar cell, comprising the steps of: providing an optical probe light; modulating the optical probe light with a modulation frequency of between 100 kHz and 50 MHz, thereby obtaining a modulated probe light; scanning the modulated probe light such that said modulated probe light is incident on at least a part of the surface of the solar cell, and such that the part of the solar cell exposed to the modulated probe light converts the modulated probe light to an electrical signal; detecting and analyzing said electrical signal; and estimating variations in the solar cell, thereby electrically characterizing the solar cell. The disclosure further relates to a solar cell characterization apparatus for characterization of a solar cell, comprising: a light source for generating an optical probe light; a modulation unit, configured to produce modulated probe light by modulating the optical probe light with a modulation frequency of between 100 kHz and 0 MHz; a light scanning unit for scanning the modulated probe light such that said modulated probe light is incident on at least a part of the surface of the solar cell; and a signal analyzer, configured to detect and analyze electrical signals produced by the solar cell as a response to exposure of the modulated probe light.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Krebs, F. C. (Intern)
Publication date: 16 Mar 2017

Publication information
IPC: H02S 50/ 15 A I
Patent number: WO2017042248
Date: 18/03/2017
Priority date: 08/09/2015
Durable fuel electrode

The present invention relates to a composite for an electrode, a composite precursor, a method of manufacturing a composite, and the composite obtained by said method. The invention further relates to an electrode comprising the composite, as well as a solid state electrochemical cell comprising the composite. The invention also relates to the use of the composite as a fuel electrode, solid oxide fuel cell, and/or solid oxide electrolyser. The invention discloses a composite for an electrode, comprising a three-dimensional network of dispersed metal particles, stabilised zirconia particles and pores, wherein the size of the pores is smaller than the size of the metal particles, wherein the size of the metal particles is essentially equal to or smaller than the size of the stabilised zirconia particles, wherein the porosity is below 33, 30, or 29 vol%, more preferably below 26 or 24 vol%, and most preferably below 23, 22, 21, 18, 15, or 13 vol%, and/or wherein the pores are essentially exclusively generated from the volume created by reducing a corresponding metal oxide to the metal particles.

3D printed barium titanate/poly-(vinylidene fluoride) nano-hybrid with anisotropic dielectric properties

Electrospun BaTiO₃ nanofibers (BTNFs) are synthesized and blended in a poly(vinylidene fluoride) (PVDF) matrix to obtain a flexible nano-hybrid composite with high dielectric constant (flexible high-k). The blending is performed with different BTNF contents (0.6, 4.5, 20 vol%). The rheological properties of the starting materials are optimized to shape the hybrid by the precision-extrusion-based fuse deposition modeling technique. The 3D-printed BTNFs allow complex shapes with different degrees of fiber alignment as the result of printing shear stress and the chemical composition of the starting material. The dielectric properties of the nano-hybrid are controlled by anisotropy with an enhancement in the nanofiber cross direction (⊥), where the dielectric constant k⊥ at 1 kHz is increased to ca. 200 from 13 of the PVDF matrix.
Acid-base chemistry and proton conductivity of CsHSO₄, CsH₂PO₄ and their mixtures with N-heterocycles

Caesium hydrogen sulfate (CsHSO₄) and caesium dihydrogen phosphate (CsH₂PO₄) are solid acids that undergo superprotonic phase-transitions at about 140 and 230 °C, respectively. As a result, the proton conductivity is increased by several orders of magnitude. However, the practical operational temperature range is narrow due to decomposition of the high-conductivity phases. For CsHSO₄, it is known that this window can be extended to lower temperatures by addition of carefully selected N-heterocycles. The present work investigates if the same approach can be used to extend the practical operating temperature range of CsH₂PO₄ as well. Binary mixtures of CsH₂PO₄ with 1,2,4-triazole, benzimidazole or imidazole were prepared by means of mechanochemical synthesis. Mixtures based on CsHSO₄ were prepared as a basis for a comparative discussion. It was found that CsHSO₄ formed organic-inorganic salts, while CsH₂PO₄ formed heterogeneous mixtures with the N-heterocycles due to its weaker acidity. At a N-heterocycle content of 30 mol%, enhanced proton conductivity was observed for both solid acids at temperatures below their superprotonic phase transitions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Gao, Y. (Intern), Han, J. (Intern), Li, Q. (Intern)
Pages: 13-19
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 306
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 2.41 SNIP 0.751 CiteScore 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
A Contribution to the Understanding of the Combined Effect of Nitrogen and Boron in Grey Cast Iron

Inoculation is an essential part of controlling material properties in grey cast iron. Inoculation practice has for decades been based on the addition to the melt of small amounts of elements with a strong affinity to O (and S) just before casting takes place. This method is proven—both in theory and in practice—to be effective in most cases. But it has the disadvantage that the nucleation effect fades away over time. In particular, in heavy castings (slow cooling) this effect may cause non-uniform and unacceptable material properties in some parts of the casting. Nitrogen is also known to influence grey iron microstructure. Both graphite flake formation and matrix formation are influenced. However, the obtained effects...
differ considerably between different reported investigations. This investigation deals with the combined effect of nitrogen and boron and how it is possible to utilize this effect to enhance material properties in heavy grey iron castings. It is shown that the controlled additions of nitrogen and boron can be used to control the microstructure of thick section grey iron castings. A plausible theory for the formation of boron nitride nuclei effective for graphite growth is presented.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Department of Mechanical Engineering, Manufacturing Engineering, Dansk Udviklings Formidling ApS
Authors: Strande, K. (Ekstern), Tiedje, N. S. (Intern), Chen, M. (Intern)
Number of pages: 10
Pages: 61-70
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Metalcasting
Volume: 11
Issue number: 1
ISSN (Print): 1939-5981
Ratings:
- Web of Science (2017): Indexed yes
- Scopus rating (2016): CiteScore 0.47 SJR 0.282 SNIP 0.672
- Scopus rating (2015): SJR 0.292 SNIP 0.59 CiteScore 0.32
- Scopus rating (2014): SJR 0.235 SNIP 0.557 CiteScore 0.37
- Scopus rating (2013): SJR 0.173 SNIP 0.332 CiteScore 0.18
- ISI indexed (2013): ISI indexed yes
- Scopus rating (2012): SJR 0.194 SNIP 0.696 CiteScore 0.31
- ISI indexed (2012): ISI indexed yes
- Scopus rating (2011): SJR 0.281 SNIP 1.021 CiteScore 0.41
- ISI indexed (2011): ISI indexed no
- Scopus rating (2010): SJR 0.257 SNIP 0.642
- Web of Science (2010): Indexed yes
- Scopus rating (2009): SJR 0.164 SNIP 0.04
- Scopus rating (2008): SJR 0.104 SNIP 0
Original language: English
Nitrogen, Boron, Control, Properties, Grey iron, Heavy castings
Electronic versions:

A_Contribution_to_the_Understanding_of_the_Combined_Effect_of_Nitrogen.pdf. Embargo ended: 30/08/2017

DOIs:
10.1007/s40962-016-0079-6
Source: FindIt
Source-ID: 2342425870
Publication: Research - peer-review › Journal article – Annual report year: 2017

**Addressing uncertainty in atomistic machine learning**

Machine-learning regression has been demonstrated to precisely emulate the potential energy and forces that are output from more expensive electronic-structure calculations. However, to predict new regions of the potential energy surface, an assessment must be made of the credibility of the predictions. In this perspective, we address the types of errors that might arise in atomistic machine learning, the unique aspects of atomistic simulations that make machine-learning challenging, and highlight how uncertainty analysis can be used to assess the validity of machine-learning predictions. We suggest this will allow researchers to more fully use machine learning for the routine acceleration of large, high-accuracy, or extended-time simulations. In our demonstrations, we use a bootstrap ensemble of neural network-based calculators, and show that the width of the ensemble can provide an estimate of the uncertainty when the width is comparable to that in the training data. Intriguingly, we also show that the uncertainty can be localized to specific atoms in the simulation, which may offer hints for the generation of training data to strategically improve the machine-learned representation.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Brown University
Authors: Peterson, A. A. (Ekstern), Christensen, R. (Intern), Khorshidi, A. (Ekstern)
Pages: 10978-10985
A Decade of Solid Oxide Electrolysis Improvements at DTU Energy

Solid oxide electrolysis cells (SOECs) can efficiently convert electrical energy (e.g., surplus wind power) to energy stored in fuels such as hydrogen or other synthetic fuels. Performance and durability of the SOEC have increased orders of magnitude within the last decade. This paper presents a short review of the R&D work on SOEC single cells conducted at DTU Energy from 2005 to 2015. The SOEC improvements have involved increasing the performance of the oxygen electrode, elimination of impurities in the feed streams, optimization of processing routes, and fuel electrode structure optimization. All together, these improvements have led to a decrease in long-term degradation rate from ~40 %/kh to ~0.4 %/kh for steam electrolysis at -1 A/cm², while the initial area specific resistance has been decreased from 0.44 Ωcm² to 0.15 Ωcm² at -0.5 A/cm² and 750 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Mixed Conductors, Imaging and Structural Analysis
Number of pages: 12
Pages: 3-14
Publication date: 2017
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 75
Issue number: 42
ISSN (Print): 1938-6737
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
A density functional theory study of the carbon-coating effects on lithium iron borate battery electrodes

Lithium iron borate (LiFeBO3) is a promising cathode material due to its high theoretical specific capacity, inexpensive components and a small volume change during operation. Yet, challenges relating to severe air- and moisture-induced degradation necessitate the application of a protective coating on the electrode which also improves the electronic conductivity. However, not much is known about the preferential geometries of the coating as well as how these coating–electrode interfaces influence the lithium diffusion between the coating and the electrode. Here, we therefore present a density functional theory (DFT) study of the anchoring configurations of carbon coating on the LiFeBO3 electrode and its implications on the interfacial lithium diffusion. Due to large barriers associated with Li-ion diffusion through a parallel-oriented pristine graphene coating on the FeBO3 and LiFeBO3 electrode surfaces, large structural defects in the graphene coating are required for fast Li-ion diffusion. However, such defects are expected to exist only in small concentrations due to their high formation energies. Alternative coating geometries were therefore investigated, and the configuration in which the graphene coating layers were anchored normal to the electrode surface at B and O atoms were found to be most stable. Nudged elastic band (NEB) calculations of the lithium diffusion barriers across the interface between the optimally oriented coating layers and the electrode show no kinetic limitations for lithium extraction and insertion. Additionally, this graphite-coating configuration showed partial blocking of electrode-degrading species.
A facile approach to fabricate hierarchically structured poly(3-hexylthiophene-2,5-diyly) films

Microstructured surfaces have great potentials to improve the performances and efficiency of optoelectronic devices. In this work, a simple robust approach based on surface instabilities was presented to fabricate poly(3-hexylthiophene-2,5-diyly) (P3HT) films with ridge-like/wrinkled composite microstructures. Namely, the hierarchically patterned films were prepared by spin coating the P3HT/tetrahydrofuran (THF) solution on a polydimethylsiloxane (PDMS) substrate to form stable ridge-like structures, followed by solvent vapor swelling to create surface wrinkles with the orientation guided by the ridge-like structures. During spin coating of the P3HT/THF solution, the ridge-like structures were generated by the in-situ template of the THF swelling-induced creasing structures on the PDMS substrate. To our knowledge, it is the first report that the creasing structures are used as a recoverable template for patterning films. The crease-templated ridge-like structures were well modulated by the THF swelling time, the modulus of the PDMS substrate, the P3HT/THF solution concentration and the selective/blanket exposure of the PDMS substrate to O2 plasma. UV–vis and fluorescence spectrometry measurements indicated that the light absorption and fluorescent emission were improved on the hierarchically patterned P3HT films, which can be utilized to enhance the efficiencies of organic solar cells. Furthermore, this simple versatile method based on the solvent swelling-induced crease as the in-situ recoverable template has been extended to pattern other spin-coated films with different compositions.
A Fully Developed Flow Thermofluid Model for Topology Optimization of 3D-Printed Air-Cooled Heat Exchangers

In this work, density-based topology optimization is applied to the design of the air-side surface of dry-cooled power plant condensers. A topology optimization model assuming a steady-state, thermally and fluid dynamically fully developed internal flow is developed and used for this application. The conductance of the heat exchanger is maximized for a prescribed pressure drop and prescribed air-side temperature change across the heat exchanger. Polymer with infilled thermally conducting metal filaments is considered as the heat exchanger material which allows cost effective additive manufacturing techniques to be used to fabricate the obtained designs. Parametric studies are presented that analyze the effect of the material thermal conductivity and the heat exchanger unit cell height on the system’s performance. The designs obtained from topology optimization are benchmarked against a simple optimized slot channel model in order to demonstrate the superior performance of the topology optimized designs. Thus, this work demonstrates the usefulness of topology optimization to fully exploit the design freedom afforded by additive manufacturing technologies.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Wisconsin-Madison
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Pages: 10-24
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 119
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.462 SNIP 1.828
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.734 SNIP 1.898 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.576 SNIP 2.206 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.516 SNIP 2.5 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.54 SNIP 2.432 CiteScore 2.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.389 SNIP 2.186 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Alkaline membrane water electrolysis with non-noble catalysts
As renewable energy sources reach higher grid penetration, large scale energy storage solutions are becoming increasingly important. Hydrogen produced with renewable energy by water electrolysis is currently the only option to solve this challenge on a global scale, and green hydrogen is essential for the decarbonization of the transportation and industrial sector required to limit climate change.

Electrolysis done with an alkaline electrolyte is a cheap, proven, and commercially available technology, but the systems suffer from inefficiency and limited operating flexibility. The work herein seek to address these issues by introducing alkaline polymeric membranes and efficient electrodes based on novel materials. Polymer electrolyte membranes with sufficient OH⁻ conductivity enable a drastic reduction of the electrode spacing, which lead to improved ohmic properties enabling operation at higher current density. This, combined with better gas separation properties and a higher operating flexibility, have the prospects of significantly reducing the capex and opex of electrolysis systems, and the cost of green hydrogen. Towards this goal, membranes based on poly(2,2'-(m-phenylene)-5,5'-bibenzimidazole) (m-PBI) as well as poly(2,2'-(m-mesitylene)-5,5'-bibenzimidazole) (mes-PBI) were investigated as electrolyte for alkaline electrolysis cells.

PBI membranes were equilibrated with aqueous KOH and applied as separator, and polarization data from cells at 20-25 wt% KOH using these membranes showed improved ohmic behaviour over cells with conventional porous separators. This was strikingly clear when combined with active electrodes with Raney-nickel-based coatings. With thin 40 μm m-PBI membranes, Raney-nickel-molybdenum cathodes and nickel anodes, cells operated at 80°C with 24 wt% KOH (aq) achieved 1000 mA cm⁻² at 1.7 V and 2800 mA cm⁻² at 2.0 V. Electrochemical impedance spectroscopy data showed a 6-fold reduction in ohmic cell resistance compared to conventional materials. Albeit good performance, ex-situ characterization and durability tests showed that polymer backbone and membrane stability remained a problem under conventional operating conditions.

To accompany novel membranes in alkaline electrolysis, electrodes can be employed in a zero-gap configuration. This enable different electrode concepts than used in commercial systems. Inspired by recent literature, nickel-iron based anodes, and nickel-tin as well as nickel-molybdenum cathodes were investigated in half cell tests. The materials were applied as coatings on nickel foam and showed improvements in the order of 150-300 mV over reference nickel materials at room temperature, depending on the specific electrode and electrolyte concentration used. In a secondary approach, electrodes were prepared using powder and polymeric binders. Using nickel powder with m-PBI binder in a nickel foam as cathode, a reduction in cell overpotential of more than 200 mV was achieved compared against a pristine nickel foam cathode.
Analysis of electrical and thermal stress effects on PCBM:P3HT solar cells by photocurrent and impedance spectroscopy modeling

We investigated the effects of electrical stress and thermal storage by means of photocurrent, Impedance Spectroscopy and Open Circuit Voltage Decay models. The electrical stress damages only the active layer, by reducing the generation rate, the polaron separation probability and the carrier lifetime. The thermal stress also degrades the anode interface. This reflects on the appearance of an inflection in the I-V photocurrent shape close to the operative region.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Torto, L. (Ekstern), Rizzo, A. (Ekstern), Cester, A. (Ekstern), Wrachien, N. (Ekstern), Passarini, L. (Ekstern), Krebs, F. C. (Intern), Corazza, M. (Intern), Gevorgyan, S. A. (Intern)
Number of pages: 10
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the IEEE International Reliability Physics Symposium (IRPS 2017)
Publisher: IEEE
Article number: 2F-4
ISBN (Print): 978-1-5090-6640-7
Analysis of Gas Leakage and Current Loss of Solid Oxide Fuel Cells by Screen Printing

Two types of anode supported solid oxide fuel cell (SOFC) NiO-YSZ/YSZ/GDC/LSCF with the same structure and different manufacturing process were tested. Gas leakage was suspected for cells manufactured with screen printing technique. Effective leak current densities for both types of cells were calculated. Their performances of electrochemical impedance spectroscopy (EIS) were compared and distribution function of relaxation times (DRT) technique was also used to find the clue of gas leakage. Finally, thinning and penetrating holes were observed in electrolyte layer, which confirmed the occurrence of gas leakage.
Analysis of Gas Leakage and Current Loss of Solid Oxide Fuel Cells by Screen Printing

One of the biggest advantages of SOFC (solid oxide fuel cell) is the probable use of methane as fuel. However, when the actual SOFC stack is operating with CH₄ as fuel, due to the catalytic action of metal nickel, carbon will deposit on SOFC anode and nickel foam, which directly shorten the SOFC operating life and lead to performance degradation. The planar anode-supported Ni-YSZ|YSZ|LSCF SOFC was chosen as the research object, with the cell size of 12cm×12cm and the effective area of 100cm², and the holder is made of 99% purity of Al₂O₃ ceramic material, in order to eliminate the influence of Cr in stainless steel. The one-cell stack operated at 750℃, and the maximum power density was 0.35W/cm² when the fuel is 0.5slm/min pure hydrogen. The stability experiment was conducted first under pure H₂ for 100h, then fuel was switched into pure methane, and another 100h of voltage stability was tested. In this work, the temperature distribution of the stack was monitored, whose relationship with the weight gain and the micro-structure of the nickel foam was established, and a possible explanation of the carbon deposition distribution and process on the nickel foam was put forward.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Tsinghua University
Authors: Jia, C. (Ekstern), Han, M. (Ekstern), Chen, M. (Intern)
Pages: 1
Publication date: 2017
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-03
Article number: 87
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org/content/MA2017-03/1/87.abstract

Bibliographical note
Poster Session I (Cathodes and Anodes)

An effective low Pd-loading catalyst for hydrogen generation from formic acid

As an interesting hydrogen carrier, formic acid is bio-renewable, non-toxic and available in the liquid state at room temperature. The development of active and low-cost catalyst is of significance for hydrogen generation from formic acid. In this study, both a relatively cheap metal (Ag) and a functional support (nitrogen modified reduced graphene oxide, N-rGO) were applied to prepare Pd catalyst. It was found that the Ag atoms facilitated the formation of Pd-rich surface in the preparation strategy, in which the reductive N-rGO and a two-step feeding process of metal precursors played important roles. In addition, Ag additive was found to benefit catalyst stability. Most interestingly, the obtained low Pd-loading Pd₁Ag₆/N-rGO catalyst showed a specific Pd loading turnover frequency of 171 mol Pd⁻¹ h⁻¹ and a specific metal cost turnover frequency of 64.2 $−1 h−1, which were predominant among currently available Pd-based catalysts towards formic acid decomposition without any additive under room temperature.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, China University of Geosciences
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Pages: 18375-18382
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 29
ISSN (Print): 0360-3199
Ratings: BFI (2018): BFI-level 1
A new method to measure mechanics and dynamic assembly of branched actin networks

We measured mechanical properties and dynamic assembly of actin networks with a new method based on magnetic microscopic cylinders. Dense actin networks are grown from the cylinders’ surfaces using the biochemical Arp2/3-
machinery at play in the lamellipodium extension and other force-generating processes in the cell. Under a homogenous magnetic field the magnetic cylinders self-assemble into chains in which forces are attractive and depend on the intensity of the magnetic field. We show that these forces, from piconewtons to nanonewtons, are large enough to slow down the assembly of dense actin networks and controlled enough to access to their nonlinear mechanical responses. Deformations are measured with nanometer-resolution, well below the optical resolution. Self-assembly of the magnetic particles into chains simplifies experiments and allows for parallel measurements. The combination of accuracy and good throughput of measurements results in a method with high potential for cell and cytoskeleton mechanics. Using this method, we observed in particular a strong nonlinear mechanical behavior of dense branched actin networks at low forces that has not been reported previously.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, ESPCI Paris, Universitat Pompeu Fabra
Authors: Bauër, P. (Ekstern), Tavacoli, J. (Intern), Pujol, T. (Ekstern), Planade, J. (Ekstern), Heuvingh, J. (Ekstern), Du Roure, O. (Ekstern)
Number of pages: 11
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 7
Article number: 15688
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.886 SNIP 1.51 CiteScore 4.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.458 SNIP 0.896 CiteScore 2.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions:
s41598_017_15638_5orb.pdf
DOIs:
10.1038/s41598-017-15638-5
Source: PublicationPreSubmission
Source-ID: 139557206
Publication: Research - peer-review › Journal article – Annual report year: 2017

Anisotropic Proton and Oxygen Ion Conductivity in Epitaxial Ba$_2$In$_2$O$_5$ Thin Films
Solid oxide oxygen ion and proton conductors are a highly important class of materials for renewable energy conversion devices like solid oxide fuel cells. Ba$_2$In$_2$O$_5$ (BIO) exhibits both oxygen ion and proton conduction, in a dry and humid environment, respectively. In a dry environment, the brownmillerite crystal structure of BIO exhibits an ordered oxygen ion sublattice, which has been speculated to result in anisotropic oxygen ion conduction. The hydrated structure of BIO,
however, resembles a perovskite and the protons in it were predicted to be ordered in layers. To complement the significant theoretical and experimental efforts recently reported on the potentially anisotropic conductive properties in BIO, we measure here both the proton and oxygen ion conductivity along different crystallographic directions. Using epitaxial thin films with different crystallographic orientations, the charge transport for both charge carriers is shown to be anisotropic. The anisotropy of the oxygen ion conduction can indeed be explained by the layered structure of the oxygen sublattice of BIO. The anisotropic proton conduction, however, further supports the suggested ordering of the protonic defects in the material. The differences in proton conduction along different crystallographic directions attributed to proton ordering in BIO are of a similar extent as those observed along different crystallographic directions in materials where proton ordering is not present but where protons find preferential conduction pathways through chainlike or layered structures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Atomic scale modelling and materials, Paul Scherrer Institute, Chalmers University of Technology, University of Göttingen, University of Verona
Authors: Fluri, A. (Ekstern), Gilardi, E. (Ekstern), Karlsson, M. (Ekstern), Roddatis, V. (Ekstern), Bettinelli, M. (Ekstern), Castelli, I. E. (Intern), Lippert, T. (Ekstern), Pergolesi, D. (Ekstern)
Pages: 21797–21805
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 121
Issue number: 40
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
A Novel Algorithm for Lifetime Extrapolation, Prediction, and Estimation of Emerging PV Technologies

Accurate determination of the lifetime of novel hybrid and organic solar cells is often rather challenging due to the very dynamic behavior of such cells over time and ageing curves with shapes of varying nature. Therefore, in order to accurately and reproducibly determine the lifetime of photovoltaic devices with such a behavior, a novel elaboration algorithm is developed, which enables automatic smoothing, filtering, and extrapolation of the real lifetime data and reproducible determination of the lifetime parameters defined in the International Summit on OPV Stability guiding standards. The algorithm is also capable of predicting the lifetime of devices, not tested until the end of sample life, given that there is sufficient number of measured data points to perform reliable extrapolation of ageing curves (to a limited time frame). The algorithm is discussed in detail and a range of examples for different lifetime data are presented.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Rizzo, A. (Ekstern), Cester, A. (Ekstern), Madsen, M. V. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. A. (Intern)
Number of pages: 9
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Small Methods
Article number: 1700285
ISSN (Print): 2366-9608
Original language: English
DOIs: 10.1021/acsjpcc.7b02497
Source: FindIt
Source-ID: 2390676972
Publication: Research - peer-review › Journal article – Annual report year: 2017

A Novel SOFC/SOEC Sealing Glass with a Low SiO2 Content and a High Thermal Expansion Coefficient

Solid oxide cells require seals that can function in harsh, elevated temperature environments. In addition, a low Si content can be advantageous, since Si impurities from the glass sealant can be transported to the active fuel electrode and poison the Ni-YSZ triple phase boundaries. To reduce the amount of Si emission, a low Si containing sealing glass (chemical composition: 50 mol% CaO, 20 mol% ZnO, 20 mol% B2O3 and 10 mol% SiO2) was developed at DTU. In this work, the results from thermal characterization, the crystallization behavior of the glass and the long-term stability and adhesion behavior of the glass were studied under SOFC and SOEC relevant conditions. The glass-ceramic sealant performed well over 400 h, and no cell degradation or leakage related to the seal was found, indicating that the developed glass system is applicable for the use in SOFC/SOEC stacks.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Kiebach, W. (Intern), Agersted, K. (Ekstern), Zielke, P. (Intern), Ritucci, I. (Intern), Brock, M. B. (Intern), Hendriksen, P. V. (Intern)
Pages: 1739-1747
A Novel SOFC/SOEC Sealing Glass with a Low SiO₂ Content and a High Thermal Expansion Coefficient

Solid oxide cells require seals that can function in harsh, elevated temperature environments. In the case of solid oxide electrolysis (SOEC), also a low Si content is desired, since Si impurities from the glass sealing can be transported to the active fuel electrode and poison the Ni-YSZ triple phase boundaries.

To reduce the amount of Si emission, a low Si containing sealing glass (chemical composition: 48 mol% CaO, 19 mol% ZnO, 21 mol% B₂O₃ and 12 mol% SiO₂) was developed at DTU. In this presentation, the results from thermal characterization, like thermal expansion coefficient, glass transition temperature, crystallization temperature, etc., of the glass will be presented. Additionally, the crystallization behavior of the glass was analyzed by in-situ X-ray diffraction, recording temperature resolved XRD spectra from 30 °C up to 900 °C.

Furthermore, the long-term stability and the adhesion behavior of the glass were studied under relevant SOFC and SOEC conditions. The stability of sealed Crofer/Glass/NiO-YSZ assemblies in reducing atmosphere and in air was investigated for over 500 h at temperatures between 750 °C and 850 °C. Additionally, a cell component test was performed to investigate the durability of the glass seal when exposed to dual atmosphere environments. The seals performed well over 400 h under fuel cell and electrolysis operation conditions, and no cell degradation or leakage related to the sealing was found, indicating that the developed glass system is applicable for the use in SOFC/SOEC stacks.
A Physically-Based Equivalent Circuit Model for the Impedance of a LiFePO4/Graphite 26650 Cylindrical Cell

In this work an Equivalent Circuit Model (ECM) is developed and used to model impedance spectra measured on a commercial 26650 LiFePO4/Graphite cylindrical cell. The ECM is based on measurements and modeling of impedance spectra recorded separately on cathode (LiFePO4) and anode (Graphite) samples, harvested from the commercial cell. Modeling of the single-electrode impedance spectra provided information about the electronic and ionic resistance in the porous composite electrodes, as well as the solid state diffusion. Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) of anode and cathode samples was used to make 3-D maps of the electrode microstructures and to obtain microstructural data for the ECM. The complementary analysis was crucial for the resolution of the single electrode impedance parameters and the proposal and validation of a new equivalent circuit used to model the full commercial battery impedance.

A Physically-Based Equivalent Circuit Model for the Impedance of a LiFePO4/Graphite 26650 Cylindrical Cell

In this work an Equivalent Circuit Model (ECM) is developed and used to model impedance spectra measured on a commercial 26650 LiFePO4/Graphite cylindrical cell. The ECM is based on measurements and modeling of impedance spectra recorded separately on cathode (LiFePO4) and anode (Graphite) samples, harvested from the commercial cell. Modeling of the single-electrode impedance spectra provided information about the electronic and ionic resistance in the porous composite electrodes, as well as the solid state diffusion. Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) of anode and cathode samples was used to make 3-D maps of the electrode microstructures and to obtain microstructural data for the ECM. The complementary analysis was crucial for the resolution of the single electrode impedance parameters and the proposal and validation of a new equivalent circuit used to model the full commercial battery impedance.
Application of numerical inverse method in calculation of composition-dependent interdiffusion coefficients in finite diffusion couples

The previously developed numerical inverse method was applied to determine the composition-dependent interdiffusion coefficients in single-phase finite diffusion couples. The numerical inverse method was first validated in a fictitious binary finite diffusion couple by pre-assuming four standard sets of interdiffusion coefficients. After that, the numerical inverse method was then adopted in a ternary Al-Cu-Ni finite diffusion couple. Based on the measured composition profiles, the ternary interdiffusion coefficients along the entire diffusion path of the target ternary diffusion couple were obtained by using the numerical inverse approach. The comprehensive comparisons between the computations and the experiments indicate that the numerical inverse method is also applicable to high-throughput determination of the composition-
dependent interdiffusion coefficients in finite diffusion couples.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Central South University
Pages: 197-211
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Metallurgical and Materials Engineering
Volume: 23
Issue number: 3
ISSN (Print): 2217-8961
Original language: English
Diffusion, Interdiffusion coefficient, Numerical inverse method, Finite diffusion couple
Electronic versions:
90_2017Liu.pdf
Links:
Source: PublicationPreSubmission
Source-ID: 140299077
Publication: Research - peer-review › Journal article – Annual report year: 2017

**Application of Photocurrent Model on Polymer Solar Cells Under Forward Bias Stress**
We performed a constant current stress at forward bias on organic heterojunction solar cells. We measured current voltage curves in both dark and light at each stress step to calculate the photocurrent. An existing model applied to photocurrent experimental data allows the estimation of several parameters such as generation, recombination, dissociation rate, and nearly zero field voltage within the active layer as a function of the stress time. The analysis of extrapolated parameters shows that the stress mainly affects the recombination rate of the polaron charge transfer states.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Rizzo, A. (Ekstern), Torto, L. (Ekstern), Wrachien, N. (Ekstern), Corazza, M. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. (Intern), Cester, A. (Ekstern)
Pages: 1542-1548
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: IEEE Journal of Photovoltaics
Volume: 6
Issue number: 6
ISSN (Print): 2156-3381
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.512 SNIP 1.58
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.909 SNIP 1.966 CiteScore 4.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.212 SNIP 1.888 CiteScore 3.87
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.357 SNIP 3.532 CiteScore 3.84
Scopus rating (2012): SJR 0.863 SNIP 2.774 CiteScore 2.2
Aqueous metal–organic solutions for YSZ thin film inkjet deposition

Inkjet printing of 8% Y2O3-stabilized ZrO2 (YSZ) thin films is achieved by designing a novel water-based reactive ink for Drop-on-Demand (DoD) inkjet printing. The ink formulation is based on a novel chemical strategy that consists of a combination of metal oxide precursors (zirconium alkoxide and yttrium salt), water and a nucleophilic agent, i.e. n-methyldiethanolamine (MDEA). This chemistry leads to metal–organic complexes with long term ink stability and high precision printability. Ink rheology and chemical reactivity are analyzed and controlled in terms of metal–organic interactions in the solutions. Thin dense nanocrystalline YSZ films below 150 nm are obtained by low temperature calcination treatments (400–500 °C), making the deposition suitable for a large variety of substrates, including silicon, glass and metals. Thin films and printed patterns achieve full densification with no lateral shrinkage and high ionic conductivity.

A regenerative elastocaloric device: Experimental results

Elastocaloric cooling and heating is an alternative cooling technology that has potential to be highly efficient and environmentally friendly. Experimental results are reported for two elastocaloric regenerators made of NiTi alloys in the form of parallel plates in two plate thicknesses. For the regenerator made of 0.2 mm plates, a maximum no-load temperature span of 17.6 K was achieved for an applied strain of 4.3 %. For the regenerator with 0.35 mm plates, a maximum temperature span of 19.9 K was reached for a strain of 3.5 %. The 0.2 mm regenerator failed after approximately 5200 cycles and the 0.35 mm regenerator failed after approximately 5500 cycles.
A simple method for preparing superconducting FeSe pellets without sealing in evacuated silica tubes

Superconducting tetragonal FeSe pellets were made by reacting mixtures of elemental Fe and Se powders in argon atmosphere without sealing in evacuated silica tubes. A simple tube furnace has been used. Although the tube's material consisted of quartz, an alumina tube could be used as well. X-ray pure samples with onset of superconducting transition between 8.0K and 8.5K were obtained under specific heat treatment conditions. Residual, unreacted Fe particles could be virtually eliminated through prolonged annealing. A key factor for the synthesis of good samples consists in using processing parameters that minimize Se losses.
Assembly Modulated by Particle Position and Shape: A New Concept in Self-Assembly

In this communication we outline how the bespoke arrangements and design of micron-sized superparamagnetic shapes provide levers to modulate their assembly under homogeneous magnetic fields. We label this new approach, ‘assembly modulated by particle position and shape’ (APPS). Specifically, using rectangular lattices of superparamagnetic micron-sized cuboids, we construct distinct microstructures by adjusting lattice pitch and angle of array with respect to a magnetic field. Broadly, we find two modes of assembly: (1) immediate 2D jamming of the cuboids as they rotate to align with the applied field (rotation-induced jamming) and (2) aggregation via translation after their full alignment (dipole-dipole assembly). The boundary between these two assembly pathways is independent on field strength being solely a function of the cuboid’s dimensions, lattice pitch, and array angle with respect to field-a relationship which we capture, along with other features of the assembly process, in a ‘phase diagram’. In doing so, we set out initial design rules to build custom made assemblies. Moreover, these assemblies can be made flexible thanks to the hinged contacts of their particle building blocks. This flexibility, combined with the superparamagnetic nature of the architectures, renders our assembly method particularly appropriate for the construction of complex actuators at a scale hitherto not possible.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, University Paris Diderot - Paris 7
Authors: Tavacoli, J. W. (Intern), Heuvingh, J. (Ekstern), Du Roure, O. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials
Volume: 10
Automated angular and translational tomographic alignment and application to phase-contrast imaging

X-ray computerized tomography (CT) is a 3D imaging technique that makes use of x-ray illumination and image reconstruction techniques to reproduce the internal cross-sections of a sample. Tomographic projection data usually require an initial relative alignment or knowledge of the exact object position and orientation with respect to the detector. As tomographic imaging reaches increasingly better resolution, thermal drifts, mechanical instabilities, and equipment limitations are becoming the main dominant factors contributing to sample positioning uncertainties that will further introduce reconstruction artifacts and limit the attained resolution in the final tomographic reconstruction. Alignment algorithms that require manual interaction impede data analysis with ever-increasing data acquisition rates, supplied by more brilliant sources. We present in this paper an iterative reconstruction algorithm for wrapped phase projection data and an alignment algorithm that automatically takes 5 degrees of freedom, including the possible linear and angular motion errors, into consideration. The presented concepts are applied to simulated and real measured phase-contrast data, exhibiting a possible improvement in the reconstruction resolution. A MATLAB implementation is made publicly available and will allow robust analysis of large volumes of phase-contrast tomography data.
Bismuth phosphates as intermediate temperature proton conductors: From polycrystalline powders to amorphous glasses

Proton conducting electrolyte materials operational in the intermediate temperature range of 200-400 °C are of special interest for applications in fuel cells and water electrolysers. Bismuth phosphates in forms of polycrystalline powders and amorphous glasses are synthesized and investigated by scanning electron microscopy, X-ray diffraction, FT-IR, thermogravimetric analysis and AC impedance. Under dry atmosphere the pure crystalline and amorphous phosphates exhibit an intrinsic conductivity of up to $10^{-5}$ S cm$^{-1}$ at 250 °C. In the presence of atmospheric humidity the conductivity of both types of phosphates is significantly enhanced, reaching about $10^{-2}$ S cm$^{-1}$ at a water vapor partial pressure above 0.5 atm. During a period of more than 100 h with four humidity cycles from zero to 0.58 atm of the water vapor partial pressure, the phosphates show good stability, suggesting the potential as an intermediate temperature electrolyte.
Bottom-Up Design of a Copper-Ruthenium Nanoparticulate Catalyst for Low-Temperature Ammonia Oxidation

A novel nanoparticulate catalyst of copper (Cu) and ruthenium (Ru) was designed for low-temperature ammonia oxidation at near-stoichiometric mixtures using a bottom-up approach. A synergistic effect of the two metals was found. An optimum CuRu catalyst presents a reaction rate threefold higher than that for Ru and forty-fold higher than that for Cu. X-ray absorption spectroscopy suggests that in the most active catalyst Cu forms one or two monolayer thick patches on Ru and the catalysts are less active once 3D Cu islands form. The good performance of the tuned Cu/Ru catalyst is attributed to changes in the electronic structure, and thus the altered adsorption properties of the surface Cu sites.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Department of Chemical and Biochemical Engineering, Atomic scale modelling and materials, Universidade de Sao Paulo, Karlsruhe Institute of Technology KIT
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
ISSN (Print): 1433-7851
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.8 SNIP 2.104
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 5.958 SNIP 2.235 CiteScore 11.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.805 SNIP 2.309 CiteScore 10.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.681 SNIP 2.204 CiteScore 10.7
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.362 SNIP 2.338 CiteScore 10.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.062 SNIP 2.387 CiteScore 10.75
ISI indexed (2011): ISI indexed yes
Due to concerns about climate change, negative environmental impacts of some fuels, and the decline in the availability of fossil fuels, renewable energy technologies are growing rapidly and becoming mature. Such technologies can provide a major share of electricity supply demand globally. However, as their market share grows, concerns about potential impacts on the stability and operation of the electricity grid, as well as economic impacts due to grid upgrading requirements, may create barriers to their future expansion, due to renewable electricity’s intermittent productions and variability. ‘Green hydrogen’ can be seen as one of the solutions to integrate high penetrations of renewables in the energy system, using both the electricity and gas networks. At present, the ‘green hydrogen’ market is small and prices are high. However, costs can be driven down by upscaling the production of equipment to mass production; supply chain optimisation, and there is also still room for technology improvement. Now is the time to prepare for the integration of significant quantities of ‘green hydrogen’ into the energy system and gain experience from large-scale demonstration of relevant hydrogen concepts.

The BIG HIT project is creating a replicable hydrogen territory in Orkney (An island archipelago six miles offshore from North of Mainland Scotland.) by implementing a fully integrated model of hydrogen production, storage, distribution of the hydrogen across Orkney and utilised for mobility, heat and power. The BIG HIT project will use otherwise curtailed electricity from one wind turbine on Shapinsay and one wind turbine and a tidal test sites on Eday, and use 1.5 MW of Polymer Electrolyte Membrane (PEM) electrolyser to convert it into ~50 t pa of hydrogen. This will be used to provide heat to local public buildings. The excess hydrogen will be transported by ferry in hydrogen tube trailers to the Orkney islands largest town, Kirkwall, where it will be used to fuel a 75 kW fuel cell stack (which will provide heat and power to ferries when docked); and the remaining hydrogen will be used at a refuelling station to fuel a fleet of up to 10 electric-hydrogen range extended vans.

The present business model report includes a financial analysis of the demonstration project and should provide an early warning if there is anything that would require the project to be altered (for example, to negotiate negative priced input electricity). By gathering and critically examining inputs from project partners and equipment suppliers: electrolyser (ITM power), tube trailer (Calvera), catalytic hydrogen (H2) boilers (Giacomini), compressor (Hofer), fuel cell stack (Arcola Energy), Hydrogen Fuel Cell (H2 FC) van (SymbioFCell) and other stakeholders, the business model is developed within
the 1st year of the project.

The cost analysis of this project considers the life cycle of hydrogen starting from the hydrogen production, transportation, and consumption. The cost includes the fixed cost for equipment and infrastructure investment and operation cost of electricity and water consumption. The functional unit is 1 kg hydrogen produced and consumed. The data collected from the project patterns and suppliers. The current analysis is based on the estimation of hydrogen production and consumption on both Shapinsay and Eday. Another objective of this report is replicability of the concept for follower territories of BIG HIT. So the cost of a replicated BIG HIT concept in the 5th year after starting BIG HIT is modelled based on the assumed capital cost reductions. Capital costs will be driven down through mass production or supply chain optimisation, and also by the technology development.

Under the two different time frames (present expectations and replication after 5 years of BIG HIT), five different scenarios are built to analyse the cost. In the first scenario S1 (current situation with limited use of curtailed energy) and the second scenario S2 (full utilisation of curtailed energy), the electrolysers on Eday and Shapinsay are directly connected to wind turbines and tidal test site. The electricity supply for the electrolyser is only from otherwise curtailed electricity. In the third scenario S3 (full utilisation of electrolysis capacity and the consumed electricity from curtailed electricity), the fourth scenario S4 (full capacity of electrolyser and electricity from both curtailed electricity and power grid), and the fifth scenario S5 (full capacity of electrolyser and the consumed electricity from power grid), the electrolysers are connected to both the wind turbines and tidal test sites and the electricity grid. In the scenarios S3, S4, and S5, it is assumed that the electrolysers can operate at full capacity and run continuously at 24 hours per day. Further it is assumed, that there is a consistent demand of ‘green hydrogen’ on the market. The difference between the otherwise curtailed electricity and grid electricity is the price. The otherwise curtailed electricity would generate an income from Feed in Tariff (FiT), which also lead to the motivation for the hydrogen producer by using the curtailed electricity. In the current BIG HIT situation (S1) the cost of hydrogen production is calculated to be 9.87 £/kg on Shapinsay and 5.17 £/kg on Eday. Two reasons cause the cost of hydrogen production to be lower on Eday than on Shapinsay. Firstly, hydrogen produced on Eday has the priority to be transported to the fuel cell in Kirkwall, which means there would be no hydrogen unconsumed on Eday. Secondly, the cost of electricity consumed by electrolyser on Eday is less than that on Shapinsay. The difference is made by Eday Renewable Energy ltd. (ERE) sharing their FiT with the project Surf n’ Turf (SnT) and the BIG HIT project where Shapinsay Renewables Limited, a child company of Shapinsay Development Trust (SDT) does not have the same agreement for the BIG HIT project by now. If the curtailed electricity from the wind turbines could be fully absorbed and the produced hydrogen would be transported and consumed consistently, the cost of producing hydrogen will decrease to 6.92 £/kg on Shapinsay if the agreement of electricity cost is same with that in S1. If the electricity cost is based on FiT, the cost of producing hydrogen will decrease to 2.52 £/kg presented in S2. With increasing of the running capacity, the cost of producing hydrogen can decrease to -2.33 £/kg with FIT support. In the replicated BIT HIT scenarios, the costs of producing hydrogen on Shapinsay are 9.02 £/kg and 2.00 £/kg in S1 and S2, respectively. If there would be no FiT for renewable electricity production in the future, the cost of hydrogen production will be 12.38 £/kg and 13.21 £/kg on Shapinsay and Eday, respectively (S5). The major cost comes from the cost of the electricity consumed from power grid. In the replicated BIT HIT project scenarios, the cost can decrease to 12.34 £/kg and 13.12 £/kg on Shapinsay and on Eday. This difference between from Shapinsay and Eday is due to the different capacity of electrolyser, 1 MW and 0.5 MW respectively.

The utilizations of hydrogen considered in this demonstration project are heat, electricity, and mobility. The replaced conventional energy sources are oil for heat, electricity from power grid, and diesel for mobility. The functional unit is defined as 1 kg hydrogen consumed. The costs of conventional fuels are obtained from the market price. The amounts of conventional fuels are calculated based on the same amounts of energy obtained from 1 kg hydrogen. The considered system boundary includes the hydrogen production process, hydrogen transportation, and hydrogen consumption. At each stage, the data has been collected from the project partners and equipment suppliers/manufacturers. The cost of hydrogen is calculated through the life cycle of hydrogen production and consumption. The suggested price of hydrogen in order to offer a cost-competitive solution is estimated. If the purpose is to supply heat (by boiler), the competitive hydrogen price is estimated to be between 1.22 £/kg and 1.28 £/kg without or with considering CO2 emission cost. If the purpose is to provide electricity and heat through a fuel cell unit, the competitive hydrogen price is between 1.48 £/kg and 2.97 £/kg without or with considering CO2 emission cost. If hydrogen is used as fuel for hydrogen fuel cell vehicles, the competitive price level of hydrogen is estimated to be 8.85 £/kg and 8.46 £/kg without or with considering CO2 emission cost.

By the comparison of the total costs for a certain heat, power or mobility service, between hydrogen technologies and conventional technologies, it is concluded that mobility is the application where hydrogen is closest to offer a cost-attractive proposition to the conventional technology, i.e. mobility using diesel as energy source. In the present scenarios, hydrogen is not close to being cost-competitive for neither heat purposes nor power purposes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Zhao, G. (Intern), Ravn Nielsen, E. (Intern)
Number of pages: 37
Publication date: 2017
Carbazole-based copolymers via direct arylation polymerization (DArP) for Suzuki-convergent polymer solar cell performance

Although direct arylation polymerization (DArP) has recently emerged as an alternative to traditional cross-coupling methods like Suzuki polymerization, the evaluation of DArP polymers in practical applications like polymer solar cells (PSCs) is limited. Because even the presence of minute quantities of defects can dramatically influence the solar cell performance, evaluation of DArP polymers offers critical insight alongside other structural and optoelectronic comparisons. Even via traditional methods, carbazole-based donors are frequently prone to homocoupling defects, which has been shown to - along with β-defects - compromise performance. Through defect minimization with the bulky and affordable neodecanoic acid (NDA) mixture, we report the synthesis of DArP poly[(9-(heptadecan-9-yl)-9H-carbazole)-alt-(4,7-di(thiophen-2-yl)benzo[1,2,5]thiadiazole)] (PCDTBT) that outperforms Suzuki PCDTBT with similar molecular weights. Expanding beyond this model system, carbazole-based polymers featuring 2,5-diethylhexyl-3,6-di(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (DPP), 4,10-bis(diethylhexyl)-thieno[2',3':5,6]pyrido[3,4-g]thieno[3,2-c]isoquinoline-5,11-dione (TPTI), 5-octyl-1,3-di(thiophen-2-yl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (DT-TPD), and 2,5-bis(2,3-dihydrothieno[3,4-b][1,4]dioxin-5-yl)pyridine (EDOT-Pyr) are generated. Polymers are characterized by 1H NMR, cyclic voltammetry, UV-Vis, GIXRD, SCLC hole mobilities, and are implemented into polymer solar cells fabricated in air under ambient humidity. We demonstrate that DArP polymers perform comparably to Suzuki in practical applications.
Carbon deposition and sulfur poisoning during CO\textsubscript{2} electrolysis in nickel-based solid oxide cell electrodes

Reduction of CO\textsubscript{2} to CO and O\textsubscript{2} in the solid oxide electrolysis cell (SOEC) has the potential to play a crucial role in closing the CO\textsubscript{2} loop. Carbon deposition in nickel-based cells is however fatal and must be considered during CO\textsubscript{2} electrolysis. Here, the effect of operating parameters is investigated systematically using simple current-potential experiments. Due to variations of local conditions, it is shown that higher current density and lower fuel electrode porosity will cause local carbon formation at the electrochemical reaction sites despite operating with a CO outlet concentration outside the thermodynamic carbon formation region. Attempts at mitigating the issue by coating the composite nickel/yttria-stabilized zirconia electrode with carbon-inhibiting nanoparticles and by sulfur passivation proved unsuccessful. Increasing the fuel electrode porosity is shown to mitigate the problem, but only to a certain extent. This work shows that a typical SOEC stack converting CO\textsubscript{2} to CO and O\textsubscript{2} is limited to as little as 15–45% conversion due to risk of carbon formation. Furthermore, cells operated in CO\textsubscript{2}-electrolysis mode are poisoned by reactant gases containing ppb-levels of sulfur, in contrast to ppm-levels for operation in fuel cell mode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Skafte, T. L. (Intern), Blennow, P. (Ekstern), Hjelm, J. (Intern), Graves, C. R. (Intern)
Pages: 54-60
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 373
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Catalyst Degradation Under Potential Cycling as an Accelerated Stress Test for PBI-Based High-Temperature PEM Fuel Cells - Effect of Humidification

In the present work, high-temperature polymer electrolyte membrane fuel cells were subjected to accelerated stress tests of 30,000 potential cycles between 0.6 and 1.0 V at 160 °C (133 h cycling time). The effect that humidity has on the catalyst durability was studied by testing either with or without humidification of the nitrogen that was used as cathode gas during cycling segments. Pronounced degradation was seen from the polarization curves in both cases, though permanent only in the humidified case. In the unhumidified case, the performance loss was more or less recoverable following 24 h of operation at 200 mA cm⁻². A difference in degradation behavior was verified with electron microscopy, X-ray diffraction, and electrochemical impedance spectroscopy. The strong effect of humidification is explained by drying of the phosphoric acid that is in the catalyst layer(s) versus maintaining humidification of this region. Catalyst degradation due to platinum dissolution, transport of its ions, and eventual recrystallization is reduced when this portion of the acid dries out. Consequently, catalyst particles are only mildly affected by the potential cycling in the unhumidified case.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems Ltd.
Authors: Søndergaard, T. (Intern), Cleemann, L. N. (Intern), Zhong, L. (Intern), Becker, H. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Seerup, L. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electro catalysis
ISSN (Print): 1868-5994
Ratings:
BFI (2018): BFI-level 1
Cathode-supported hybrid direct carbon fuel cells

The direct conversion of coal to heat and electricity by a hybrid direct carbon fuel cell (HDCFC) is a highly efficient and cleaner technology than the conventional combustion power plants. HDCFC is defined as a combination of solid oxide fuel cell and molten carbonate fuel cell. This work investigates cathode-supported cells as an alternative configuration for HDCFC, with better catalytic activity and performance. This study aims to define the best processing route to manufacture highly efficient cathode-supported cells based on La0.75Sr0.25MnO3/yttria-stabilized zirconia infiltrated backbones. The challenges on the development of high-performance backbones are discussed. In this study, cathode-supported configuration was confirmed to be more efficient for the oxidation of carbon than anode supported configuration. The maximum power density of the cathode-supported cell increased almost by a factor of two when compared with the anode-supported cell.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry
Authors: Gil, V. (Intern), Gurauskis, J. (Intern), Deleebeeck, L. (Intern), Stamate, E. (Intern), Kammer Hansen, K. (Intern)
Pages: 4311-4319
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 7
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.142 SNIP 1.286
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.294 SNIP 1.319 CiteScore 3.46
Cathodic protection of all-solid-state LiS batteries by magnetron sputtering with lithium phosphorous oxynitride

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Blanchard, D. (Intern), Stamate, E. (Intern)
Number of pages: 2
Publication date: 2017

Host publication information
Title of host publication: Nordic Battery Conference 2017 - Book of abstracts- poster presentations
Challenges and Possibilities of EIS on PEMEC

Electrochemical impedance spectroscopy (EIS) has been proven a very strong electrochemical characterization tool in electrochemical research in general and in the areas of fuel cell and battery research in particular. However, this is not the case for polymer electrolyte membrane electrolysis cells (PEMCE), for which relatively few reports on the application of systematic EIS studies are available. Asking experienced researchers in the field about why, the answer has often been that these cells reveal too much electrical noise to obtain EIS with acceptable quality due to O₂ and H₂ bubble formation. Our view of the ideal structure of a PEMEC is that there ought not to be any effect of gas bubbles on the EIS as the current paths should not be disturbed by bubbles. However, we also see noise in our spectra, but the level of noise varies very much from one cell type to another. We have studied noise on three types of PEMEC and two type of alkaline electrolysis cell (AEC) for comparison. A characteristic feature of the studied PEMEC is that there is no or very little noise seen in the EIS in the frequency range above ca. 500 Hz and again not much noise below 5 Hz.

Our hypothesis is that this phenomenon is related to bubbles that are adhering to active sites of the electrocatalyst. When the catalyst layer is subjected to alternating current (AC) during the EIS then, in the PEMEC case, the O₂ pressure and volume of the bubbles growing on the catalyst layer will oscillate with the frequency of the AC. The volume change will naturally change with the frequency. The longer the wave period (the lower the frequency) is, the bigger is the change in the amount of O₂ production during an AC period. In other words, a vibration of the O₂ bubble size and internal pressure must be induced by the AC current. Thus, we imagine that at some low frequency, the bubbles adhering to the catalytic layer get more unstable and detach with an uneven rate from the catalyst surface. This causes the noise observed. Presumably, the structure and the properties of the interface of the catalyst to the liquid aqueous phase as well as the operation parameter will affect the frequency range and the size of noise in the EIS.
Charge transport and structure in semimetallic polymers

Owing to changes in their chemistry and structure, polymers can be fabricated to demonstrate vastly different electrical conductivities over many orders of magnitude. At the high end of conductivity is the class of conducting polymers, which are ideal candidates for many applications in low-cost electronics. Here, we report the influence of the nature of the doping anion at high doping levels within the semi-metallic conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) on its electronic transport properties. Hall effect measurements on a variety of PEDOT samples show that the choice of doping anion can lead to an order of magnitude enhancement in the charge carrier mobility >3 cm²/Vs at conductivities approaching 3000 S/cm under ambient conditions. Grazing Incidence Wide Angle X-ray Scattering, Density Functional Theory calculations, and Molecular Dynamics simulations indicate that the chosen doping anion modifies the way PEDOT chains stack together. This link between structure and specific anion doping at high doping levels has ramifications for the fabrication of conducting polymer-based devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of South Australia, Linkoping University
Pages: 97-104
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Polymer Science. Part B, Polymer Physics
Volume: 56
Issue number: 1
ISSN (Print): 0887-6266
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 1.051 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.241 SNIP 1.119 CiteScore 3.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.498 SNIP 1.423 CiteScore 3.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.177 SNIP 1.313 CiteScore 3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.059 SNIP 1.158 CiteScore 2.29
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.783 SNIP 0.905 CiteScore 1.74
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.899 SNIP 0.958
Chemical and Electrochemical Properties of La\textsubscript{0.58}Sr\textsubscript{0.4}Fe\textsubscript{0.8}Co\textsubscript{0.2}O\textsubscript{3-δ} (LSCF) Thin Films upon Oxygen Reduction and Evolution Reactions

The Oxygen Evolution and Oxygen Reduction Reactions (OER/ORR), occurring at the oxygen electrode of Solid Oxide Cells (SOCs) in the two possible ways of operation, require substantial overpotentials, therefore lowering the operating efficiency of the cells. The reaction mechanisms occurring at these electrodes are still not completely understood due to their complexity and localized character at the interfaces between different materials or between the gas atmosphere and the electrocatalyst, and need in situ techniques with very high chemical sensitivity, with the additional difficulty of probing the materials as close as possible to their realistic operating conditions. In addition, the properties of LSCF are, despite numerous studies, still unclear in many aspects, despite LSCF being one of the state-of-the-art electrocatalysts used for SOCs. It is understood that the surface chemical composition deviates from the nominal bulk composition, and that secondary phases can segregate at the surfaces and interfaces during operation. Furthermore, the electrochemical properties such as Area Specific Resistance (ASR), oxygen exchange coefficient (\(k_{\text{ex}}\)), ASR activation energy (\(E_a\)) and \(pO_2\) exponents for LSCF reported in the literature vary considerably. This study aims to better understand the properties of LSCF, by combining the results of Electrochemical Impedance Spectroscopy (EIS) and Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) on model electrodes, both in polarized and unpolarized conditions. In particular, NAP-XPS studies of the surface chemistry evolution under operation, as well as the correlation between surface potential changes in relation to the applied overpotential are addressed, in an attempt to determine the real driving force for the oxygen reactions. For this purpose, thin films of LSCF are deposited by Pulsed Laser Deposition (PLD) through shadow masks, in order to obtain well-defined electrode geometries with low risk of contamination, and subsequently tested both in highly clean EIS measuring setups and at the synchrotron beamline. The results of both kinds of experiments are correlated, the goal being a better understanding of the material’s properties under operation, as well as possible degradation phenomena.
Chemical and Electrochemical Properties of La$_{0.58}$Sr$_{0.4}$Fe$_{0.8}$Co$_{0.2}$O$_{3-\delta}$ (LSCF) Thin Films upon Oxygen Reduction and Evolution Reactions

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Chemistry, Stanford University
Pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Chemical solution deposition on textured metal substrates: Enabling sustainability with large-scale and flexible functional thin films

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Ceramic Engineering & Science
Authors: Grivel, J. (Intern), Thydén, K. T. S. (Intern), Bowen, J. R. (Intern), Bjørnetun Haugen, A. (Intern), Wulff, A. C. (Intern), Yue, Z. (Intern)
Number of pages: 1
Publication date: 2017

Coarsening of carbon black supported Pt nanoparticles in hydrogen
This study addresses coarsening mechanisms of Pt nanoparticles supported on carbon black in hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H2/Ar while ramping up the temperature to almost 1000 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in a hydrogen environment are stable up to ca. 800 °C at a heating rate of 10 °C/min. The coarsening above this temperature is dominated by the particle migration and coalescence mechanism. However, for agglomerated Pt nanoparticles, coalescence events were observed already above 200 °C. The temperature-dependency of particle sizes and the observed migration distances are described and found to be consistent with simple early models for the migration and coalescence.
Commercial alkaline earth boroaluminosilicate glasses for sealing solid oxide cell stacks. Part I: Development of glass-ceramic microstructure and thermomechanical properties

Sealing performance in solid oxide cell (SOC) stacks and the devitrification process of commercially available alkaline earth boroaluminosilicate glasses containing 48-61 mol\% SiO₂, 18-28 mol\% CaO, 1-7 mol\% MgO, 7-10 mol\% Al₂O₃, 1-11 mol\% B₂O₃ plus minor amounts of Na₂O, K₂O, FeO, and TiO₂ were investigated and quantified through analysis of phase assemblages as function of heat treatments above the glass transition temperatures using the electron microprobe and powder X-ray diffraction. For two of these glasses devitrification behavior was compared to the devitrification behavior of similar glasses produced in the laboratory. Glasses were characterized after annealing in air at 800°C and 850°C for up to 6 weeks. Even though the glasses lie within a relatively narrow compositional range, sealing performance and the resulting microstructures differed significantly. Best thermomechanical properties was developed in one of the laboratory-produced glasses, MCAS, which may be applied in SOC-stacks by allowing for a slow solidification in the range 750-800°C followed by crystallization at or slightly above 800°C. The relatively high thermal expansion coefficient (CTE) from RT-800°C, 11 × 10⁻⁶ K⁻¹, which was developed over ~1000 hours at 800°C, depends mainly on the formation of cristobalite and quartz as well as the presence of a residual glass phase. The glass ceramic sealant appears relatively stable over time, except for a slow transition of cristobalite to quartz, and can possibly show self-healing behavior if later brought close to 850°C. Devitrification led to increases of the thermal expansion coefficients in all other glasses tested, but did not reach levels interesting for SOC-stack sealing.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Copenhagen
Authors: Agersted, K. (Ekstern), Balic-Zunic, T. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Applied Ceramic Technology
ISSN (Print): 1546-542X
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.08 SJR 0.396 SNIP 0.674
Scopus rating (2015): SJR 0.447 SNIP 0.866 CiteScore 1.28
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.526 SNIP 1.067 CiteScore 1.45
Scopus rating (2013): SJR 0.587 SNIP 1.004 CiteScore 1.33
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.576 SNIP 0.877 CiteScore 1.27
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 0.622 SNIP 1.117 CiteScore 1.37
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.703 SNIP 1.131
Commercial alkaline earth boroaluminosilicate glasses for sealing solid oxide cell stacks Part II: Characterization of devitrification and glass-ceramic phase assemblages

The devitrification process and formation of crystalline phases from commercial alkaline earth boroaluminosilicate glasses containing 48-61 mol% SiO$_2$, 18-28 mol% CaO, 1-7 mol% MgO, 7-10 mol% Al$_2$O$_3$, 1-11 mol% B$_2$O$_3$ plus minor amounts of Na$_2$O, K$_2$O, FeO and TiO$_2$ were quantified through analysis of phase assemblages as function of heat treatments above the glass transition temperatures using the electron microprobe and powder X-ray diffraction. Treatments at 800 °C and 850 °C lasted up to 6 weeks.

Results indicate that devitrification was strongly activated through presence of heterogeneous nucleation, and that the growth mechanism gradually changed from three-dimensional growth at the onset of devitrification towards one-dimensional growth in later stages, when heterogeneous nucleation was absent or less dominating.

Most glasses developed entangled and fibrous microstructures with little or no residual glass phase, which are adequate for rigid sealants, and only one of the laboratory analogue glasses, MCAS, developed microstructures with both more equiaxed grains and a considerable amount of residual glass phase, which may be adequate for more compliant and self-healing sealants as often required in SOC-applications.

Even though the glasses lie within a relatively narrow compositional range, resulting phase assemblages differed significantly. Anorthite (plagioclase) developed as the main crystalline phase in all samples together with pyroxene (or pyroxenoide) and cristobalite. Calcium-magnesium-silicate pyroxene (diopside) was in a large part replaced by the calcium-silicate pyroxenoide (wollastonite) in the samples where the mol-proportion MgO:CaO was 1:5 or lower. In samples with a very low MgO proportion and consequently a high CaO proportion, calcium metaborate and calcium aluminum borosilicate (okayamalite) crystallized among the main phases and these glasses crystallized completely within the period of heat treatment. Although cristobalite is metastable at the annealing temperatures, both α and β forms were rapidly formed in most of the samples, likely due to kinetic reasons. The presence of the latter is explained by the stabilization effect of Al and B substitution for Si compensated by Ca stuffing in the structure. The stuffed cristobalite transformed with time to quartz (at 800 °C) or quartz plus tridymite (at 850 °C). Boron was incorporated in the first crystallizing phases, especially diopside, substituting for Al and Si, but the so established substitution partly disappeared with time during the heat treatment.
Comminution of B₄C powders with a high-energy mill operated in air in dry or wet conditions and its effect on their spark-plasma sinterability

The comminution of a typical submicrometre B₄C powder with a high-energy mill (i.e., a shaker mill) operated in air in either a dry or a wet environment was investigated. It was found that dry shaker milling (i.e., high-energy ball-milling) is able to progressively refine the B₄C particles to the nanoscale. While this is accompanied by oxidation and aggregation, these are not serious drawbacks. Wet shaker milling in methanol (i.e., conventional ball-milling) resulted only in a moderate B₄C particle refinement with greater contamination by the milling tools, which limits its usefulness. It was also found that both dry and wet milling modify the B₄C crystal structure, attributable to carbon enrichment. Consequently, dry shaker milling was found to be more recommendable than wet shaker milling to provide B₄C starting powders with superior sinterability. A comparative densification study by spark-plasma sintering confirmed this recommendation, and also showed the usefulness of dry shaker milling to obtain refined B₄C microstructures for structural applications.
Comparative DFT+U and HSE Study of the Oxygen Evolution Electrocatalysis on Perovskite Oxides

The most common method for incorporating strong electron correlations is either to apply the Hubbard U correction on top of standard density functional theory calculations (DFT) or to use hybrid functionals. In this study, we elucidate the sensitivity of the Hubbard U correction in the PBE+U functional and the amount of exact exchange, $\alpha$, in the hybrid HSE functional on the structural stability, catalytic activity and electronic conductivity of pure and doped perovskite oxides, $\text{ABO}_3$ (A = La, Ca, Sr and Ba, B = Cr, Mn, Fe, Co, Ni and Cu) for oxygen evolution electrocatalysis. We find a strong dependence of heat of formations and reaction overpotentials for a range of $U = 0$, 3 and 5 eV and $\alpha = 0$, 0.15, 0.25, 0.35 values investigated in this study, which we attribute primarily to changes in the oxidation state of B cations. If the valence of B cations in the perovskite and reference oxide is the same, then the U- and $\alpha$ dependence is very small. On the other hand, if the valences are different then heat of formations can change by as much as 1 eV. As the oxidation state of a surface metal ion depends on adsorbed intermediate and nature of the element, similar differences in energies appear in the calculated reaction overpotentials for oxygen evolution. The large U and $\alpha$ dependence sets serious constraints on the use of DFT+U and HSE methods for assessing stabilities and catalytic activities of perovskite oxides. In addition, the large $\alpha$ dependence raises the question whether HSE calculations can improve sufficiently the accuracy of DFT+U results for multi-step electrochemical reactions to justify the excess computational cost. Although we have investigated only one particular class of catalysts and one electrochemical reaction, the results of this study can expectedly be generalized to other strongly correlated systems in which the oxidation state of the surface changes during reaction. The influence of U on the electronic conductivity is significant only in cases where it qualitatively changes the electronic structure, by e.g. opening the band-gap. From a combinatorial analysis on pure and doped oxides, we identify electronically conductive catalysts classified according to different electron conduction types: intrinsic conductivity (Fe$^{4+}$, Co$^{3+}$ (intermediate spin, IS) and Ni$^{3+}$), electron polaron hopping (along Mn$^{3+}$-O-Mn$^{4+}$ chains) and charge transport through holes in the valence band.
Comparison of iron and copper doped manganese cobalt spinel oxides as protective coatings for solid oxide fuel cell interconnects

MnCo$_2$O$_4$, MnCo$_{1.7}$Cu$_{0.3}$O$_4$, and MnCo$_{1.7}$Fe$_{0.3}$O$_4$ are investigated as coatings for corrosion protection of metallic interconnects in solid oxide fuel cell stacks. Electrophoretic deposition is used to deposit the coatings on Crofer 22 APU alloy. All three coating materials reduce the parabolic oxidation rate in air at 900 °C and 800 °C. At 700 °C there is no significant difference in oxidation rate between coated samples and uncoated pre-oxidized Crofer 22 APU. The cross-scale area specific resistance (ASR) is measured in air at 800 °C using La$_{0.85}$Sr$_{0.15}$Mn$_{1.1}$O$_3$ (LSM) contact plates to simulate the interaction with the cathode in a SOFC stack. All coated samples have three times lower ASR than uncoated Crofer 22 APU after 4370 h aging. The ASR increase with time is lowest with the MnCo$_2$O$_4$ coating, followed by the MnCo$_{1.7}$Fe$_{0.3}$O$_4$ and MnCo$_{1.7}$Cu$_{0.3}$O$_4$ coatings. LSM plates contacted to uncoated Crofer 22 APU contain significant amounts of Cr after aging, while all three coatings effectively prevent Cr diffusion into the LSM. A complex Cr-rich reaction layer develops at the coating-alloy interface during oxidation. Cu and Fe doping reduce the extent of this reaction layer at 900 °C, while at 800 °C the effect of doping is insignificant.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Norwegian University of Science and Technology
Authors: Talic, B. (Intern), Molin, S. (Intern), Wiik, K. (Ekstern), Hendriksen, P. V. (Intern), Lein, H. L. (Ekstern)
Pages: 145-156
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 372
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.968 SNIP 1.726
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.597 SNIP 1.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.8 SNIP 2.224
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.65 SNIP 1.825
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.852 SNIP 1.818
Scopus rating (2003): SJR 1.66 SNIP 1.583
Scopus rating (2002): SJR 1.959 SNIP 1.4
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.115 SNIP 1.492
Scopus rating (2000): SJR 1.106 SNIP 0.914
Scopus rating (1999): SJR 0.854 SNIP 0.998
Original language: English
Solid oxide fuel cell, Metallic interconnect, Manganese cobalt spinel, Coating, High temperature oxidation, Area specific resistance
DOIs:
10.1016/j.jpowsour.2017.10.060
Source: FindIt
Source-ID: 2392778891
Publication: Research - peer-review › Journal article – Annual report year: 2017

Computational High-throughput Screening for Solar Energy Materials

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Atomic scale modelling and materials, Theoretical Atomic-scale Physics
Authors: Castelli, I. E. (Intern), Thygesen, K. S. (Intern), Jacobsen, K. W. (Intern)
Number of pages: 30
Publication date: 2017

**Host publication information**
Title of host publication: Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications
Publisher: CRC Press
ISBN (Print): 9781498750783
Main Research Area: Technical/natural sciences
Publication: Research › Book chapter – Annual report year: 2017

Computational screening of doped αMnO2 catalysts for the oxygen evolution reaction
Minimizing energy and materials costs for driving the oxygen evolution reaction (OER) is paramount for the commercialization of water electrolysis cells and rechargeable metal-air batteries. Using density functional theory calculations, we analyze the structural stability, catalytic activity and electronic conductivity of pure and doped αMnO2 for the OER. As a model surface, we investigate the (110) and (100) facets, on which we identify three possible active sites: a coordination unsaturated, bridge and bulk site. We evaluate the performance of pure and Cr, Fe, Co, Ni, Cu, Zn, Cd, Mg, Al, Ga, In, Sc, Ru, Rh, Ir, Pd, Pt, Ti, Zr, Nb and Sn doped αMnO2. At each site and for each dopant, we impose the preferred valence by adding/subtracting electron donors (hydrogens) and electron acceptors (hydroxyls). From a subset of stable dopants, we identify Pd doped αMnO2 as the only catalyst that can outperform pristine αMnO2. We also discuss approaches to increase the electron conductivity as pure αMnO2 is a narrow band-gap material.

**General information**
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 24
Carbon black, a state-of-the-art cathode material for proton exchange membrane fuel cells (PEMFCs), suffers from severe corrosion in practical applications. Niobium-doped tin dioxide (NTO) is a promising alternative to support the Pt catalysts at the cathodes. Here, through a combined density functional theory and non equilibrium Green's function study, we investigate the Nb segregation at Pt/NTO interfaces under operational electrochemical conditions, and reveal the resulting effects on the electronic transport, as well as the catalytic properties. We find that the Nb dopants tend to aggregate in the subsurface layers of the NTO substrate, whereas their transport across the Pt/NTO interface is hindered by a high thermodynamic barrier under the operating condition of PEMFCs. The interfacial transport of Sn is, however, more facile, indicating possible formations of Sn Pt alloys and tin oxides. The electronic conductivities of the Pt/NTO systems are not
particularly sensitive to the distance of the Nb dopants relative to the interface, but depend explicitly on the Nb concentration and configuration. Through a dopant induced ligand effect, the NTO substrates can improve the catalytic activity of the Pt adsorbate toward the oxygen reduction reaction. We also investigate the co-doped SnO2 substrates by both Nb and Sb elements, and find that a small amount of Nb dopants could further improve the electronic transport of the Pt/Sb-doped-SnO2 interface. The fundamental understanding generated here will help shed light on future applications of Nb-doping and Nb-Sb co-doping in Pt/SnO2 type cathodes for PEMFC applications.
Concentration Impedance in Testing of Solid Oxide Cells Revisited

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Innovation Fund Denmark
Number of pages: 1
Publication date: 2017

**Host publication information**

Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: Electrochemical Society, Incorporated
Article number: 271
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/271

Concentration Impedance in Testing of Solid Oxide Cells Revisited

The concentration impedance originating from diffusion and reactant conversion impedance of the Ni-YSZ supported fuel electrode in solid oxide cell has been treated many times during the latest couple of decades. In spite of this, the separation of the diffusion impedance from the conversion impedance is still not trivial. Therefore, combined theoretical and experimental methods available for breakdown of the concentration impedance are outlined and discussed.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Pages: 2133-2139
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: ECS Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
Conjugated Polymers Via Direct Arylation Polymerization in Continuous Flow: Minimizing the Cost and Batch-to-Batch Variations for High-Throughput Energy Conversion

Continuous flow methods are utilized in conjunction with direct arylation polymerization (DArP) for the scaled synthesis of the roll-to-roll compatible polymer, poly[(2,5-bis(2-hexyldecyloxy)phenylene)-alt-(4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole)] (PPDTBT). PPDTBT is based on simple, inexpensive, and scalable monomers using thienyl-flanked benzothiadiazole as the acceptor, which is the first β-unprotected substrate to be used in continuous flow via DArP, enabling critical evaluation of the suitability of this emerging synthetic method for minimizing defects and the scaled synthesis of high-performance materials. To demonstrate the usefulness of the method, DArP-prepared PPDTBT via continuous flow synthesis is employed for the preparation of indium tin oxide (ITO)-free and flexible roll-coated solar cells to achieve a power conversion efficiency of 3.5% for 1 cm² devices, which is comparable to the performance of PPDTBT polymerized through Stille cross coupling. These efforts demonstrate the distinct advantages of the continuous flow protocol with DArP avoiding use of toxic tin chemicals, reducing the associated costs of polymer upscaling, and minimizing batch-to-batch variations for high-quality material.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Southern California, Technical University of Denmark
Authors: Gobalasingham, N. S. (Ekstern), Carlé, J. E. (Intern), Krebs, F. C. (Intern), Thompson, B. C. (Ekstern), Bundgaard, E. (Intern), Helgesen, M. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecular Rapid Communications
Volume: 38
Issue number: 22
Article number: 1700526
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials for Energy Conversion Devices

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Xu, Y. (Intern), Zielke, P. (Intern), Kiebach, W. (Intern)
Number of pages: 1

Conjugated polymers, Continuous flow synthesis, Direct arylation polymerization, Organic solar cells

DOI: 10.1002/marc.201700526
Source: FindIt
Source-ID: 2391893902
Publication: Research - peer-review › Journal article – Annual report year: 2017
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials Used in Energy Conversion Devices

Continuous hydrothermal flow synthesis (CHFS) was used to prepare functional oxide nanoparticles. Materials synthesized include NiO, Y-doped ZrO2, LaCrO3 and Ni-substituted CoFe2O4. These types of oxides can be applied in several energy conversion devices, e.g. as active materials in solid oxide fuel cells (SOFCs), oxygen transport membranes (OTMs), and water electrolysis processes. Compared with other chemical synthesis methods, CHFS is advantageous for preparing nanosized materials with a narrow size distribution and a high phase purity. Moreover, CHFS has a high throughput as materials are continuously produced, and the technology can be scaled-up to an industrial-relevant production capacity.

The thesis starts with investigating the most appropriate mixer design for a novel two-stage reactor by computational fluid dynamics modelling. On basis of the modelling results, a two-stage CHFS reactor was constructed, and proof-of-concept syntheses of NiO and Y-doped ZrO2 (YSZ), in both one-stage and two-stage modes, were conducted. Secondly, Gd-doped CeO2 (GDC) nanoparticles (6 – 40 nm) were synthesized, and the effect of the pH on their size, morphology and composition was studied. An up-scaled synthesis of Gd0.2Ce0.8O2-δ nanoparticles was made, and the as-synthesized particles were processed into inks that displayed a good printability in inkjet printing of electrolytes on both green NiO-GDC and pre-sintered NiO-YSZ substrates. Particularly on the pre-sintered NiO-YSZ substrate, dense continuous layers (< 2 μm in thickness) composed of GDC and YSZ that fully covered the substrate were obtained after firing at 1300 °C.

In addition, (La0.6Sr0.4)0.99CoO3 – Gd0.2Ce0.8O2-δ (LSC-GDC) core-shell type particles were prepared and their high-temperature microstructural evolution was studied in two different sintering processes, i.e. spark plasma sintering and conventional sintering. By conventional hydrothermal batch-type synthesis, a core-shell structure was realized by precipitating ~6 nm large GDC particles on the surface of LSC particles under a mild hydrothermal condition of 100 °C resulting in an integral GDC shell around the LSC core. It was found that by spark plasma sintering, a fine microstructure containing nanograins could be obtained and the graded core-shell architecture could be partially maintained.

For the first time, phase-pure LaCrO3 was obtained by CHFS without any post treatments. A continuous production of cube-shaped LaCrO3 particles (639 nm) was achieved. Processing parameters (temperature and alkali concentration) were found to affect the phase purity of the obtained particles significantly. The synthesized LaCrO3 particles were used to prepare 10Sc1YSZ – LaCrO3 dual-phase oxygen transport membranes. A density of ~90 % was achieved after firing at 1400 °C, which is below normal sintering temperatures for LaCrO3-based ceramics. Oxygen permeation fluxes up to 5 × 10−8 mol cm−2 s−1 were obtained with a 1 mm thick membrane tested in air/N2 at 900 °C.

Finally, CoFe2O4 and Ni-substituted CoFe2O4 nanoparticles were prepared by CHFS and their catalytic properties were evaluated. The CoFe2O4 was found to be active for catalytic CO oxidation. A 50 % conversion of CO at 223 °C and a complete conversion at 310 °C was reached. By CHFS, Ni-substituted CoFe2O4 nanoparticles with controlled Ni contents were synthesized, and their activity as catalysts for the oxygen evolution reaction (the half reaction of water electrolysis) was evaluated. Whereas no simple correlation between the activity and the Ni content was detected, a remarkable improvement of the activity was observed for the sample with 30 at% (in atomic percent) Ni-substituted CoFe2O4 (Co0.7Ni0.3Fe2O4) compared to all other investigated compositions.

Overall, the thesis demonstrates the versatility of the CHFS route for preparing functional oxides in nano particulate form, and documents the properties of the synthesized materials in a number of specific applications (fuel cells, membranes and catalysis).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Xu, Y. (Intern), Kiebach, W. (Intern), Hendriksen, P. V. (Intern), Norby, P. (Intern), Simonsen, S. B. (Intern)
Number of pages: 236
Publication date: 2017
Continuous Hydrothermal Flow Synthesis of Gd-doped CeO₂ (GDC) Nanoparticles for Inkjet Printing of SOFC Electrolytes

Gd₅Ce₁₋ₓO₂₋₅ (GDC) nanoparticles were synthesized using continuous hydrothermal flow synthesis. By varying the synthesis conditions, particle size and morphology could be tailored. Here, particle sizes between 6 to 40 nm with polyhedral or octahedral shape could be obtained. Gd₀.₂Ce₀.₈O₂₋₅ nanoparticles were further processed into inks for inkjet printing. Despite the small particle size/large surface area, inks with excellent printing behavior were formulated. For proof-of-concept, thin GDC layers were printed on a) green NiO-GDC substrates, and on b) pre-sintered NiO-YSZ substrates. While no dense layers could be obtained on the green NiO-GDC substrates, GDC nanoparticles printed on NiO-YSZ substrates formed a dense continuous layer after firing at 1300 °C.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Applied Electrochemistry, Imperial College London
Authors: Xu, Y. (Intern), Farandos, N. M. (Ekstern), Rosa, M. (Intern), Zielke, P. (Intern), Esposito, V. (Intern), Hendriksen, P. V. (Intern), Jensen, S. H. (Intern), Li, T. (Ekstern), Kelsall, G. H. (Ekstern), Kiebach, W. (Intern)
Number of pages: 34
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Applied Ceramic Technology
ISSN (Print): 1546-542X
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.08 SJR 0.396 SNIP 0.674
Scopus rating (2015): SJR 0.447 SNIP 0.866 CiteScore 1.28
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.526 SNIP 1.067 CiteScore 1.45
Scopus rating (2013): SJR 0.587 SNIP 1.004 CiteScore 1.33
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.576 SNIP 0.877 CiteScore 1.27
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 0.622 SNIP 1.117 CiteScore 1.37
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.703 SNIP 1.131
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.851 SNIP 1.137
Scopus rating (2008): SJR 0.974 SNIP 1.427
Scopus rating (2007): SJR 0.7 SNIP 1.249
Scopus rating (2006): SJR 0.858 SNIP 1.767
Scopus rating (2005): SJR 0.589 SNIP 1.68
Original language: English
Continuous flow synthesis, Hydrothermal, Supercritical water, Gadolinium doped ceria, Inkjet printing, SOFC, Electrolyte, Solid oxide fuel cell

DOI:
10.1111/ijac.12845
Source: PublicationPreSubmission
Source-ID: 140596701
Publication: Research - peer-review › Journal article – Annual report year: 2017
Controlling the Carrier Density of SrTiO₃-Based Heterostructures with Annealing

The conducting interface between the insulating oxides LaAlO₃ (LAO) and SrTiO₃ (STO) displays numerous physical phenomena that can be tuned by varying the carrier density, which is generally achieved by electrostatic gating or adjustment of growth parameters. Here, it is reported how annealing in oxygen at low temperatures (T < 300 °C) can be used as a simple route to control the carrier density by several orders of magnitude. The pathway to control the carrier density relies on donor oxidation and is thus applicable to material systems where oxygen vacancies are the dominant source of conductivity. Using STO capped with epitaxial γ-Al₂O₃ (GAO) or amorphous LAO (a-LAO), the pathways for changing the carrier density in the two STO-based cases are identified where oxygen blocking (GAO) and oxygen permeable (a-LAO) films create interface conductivity from oxygen vacancies located in STO near the interface. For a-LAO/STO, the rate limiting step (Eₐ = 0.25 eV) for oxidizing oxygen vacancies is the transportation of oxygen from the atmosphere through the a-LAO film, whereas GAO/STO is limited by oxygen migration inside STO (Eₐ = 0.5 eV). Finally, it is showed how the control of the carrier density enables writing of conducting nanostructures in γ-Al₂O₃/STO by conducting atomic force microscopy.

Correction: Large-scale electricity storage utilizing reversible solid oxide cells combined with underground storage of CO₂ and CH₄

Correction for 'Large-scale electricity storage utilizing reversible solid oxide cells combined with underground storage of CO₂ and CH₄' by S. H. Jensen et al., Energy Environ. Sci., 2015, 8, 2471–2479.
Corrigendum to "Model for solid oxide fuel cell cathodes prepared by infiltration" [Electrochim. Acta 229 (March (1)) (2017) 73-95]
Authors regret to inform that there was an error in Fig. 4 (equivalent circuit) of the manuscript. The correct equivalent circuit is shown below.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Samson, A. J. (Intern), Søgaard, M. (Intern), Hendriksen, P. V. (Intern)
Pages: 220
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochimica Acta
Volume: 256
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.651 SNIP 1.592 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.621 SNIP 1.803 CiteScore 4.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.691 SNIP 1.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.536 SNIP 1.625
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.533 SNIP 1.47
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.563 SNIP 1.595
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.534 SNIP 1.736
Web of Science (2006): Indexed yes
Cost-competitiveness of organic photovoltaics for electricity self-consumption at residential buildings: A comparative study of Denmark and Greece under real market conditions

To address sustainability challenges, photovoltaics (PV) are regarded as a promising renewable energy technology. Decreasing PV module costs and increasing residential electricity prices have made self-consumption of PV-generated electricity financially more attractive than exporting to the grid. Organic photovoltaics (OPV) are an emerging thin-film PV technology that shows promise of greatly improving the environmental and economic performances of PV technologies. Previous studies have estimated the current and future costs of OPV technologies, but the attractiveness of investing in OPV systems has not been evaluated under real market conditions, especially under PV self-consumption schemes. In this study, we investigate the self-consumption of electricity generation from conventional and organic PV systems installed at residential houses in two different countries, Denmark and Greece, under current PV regulatory frameworks. We then focus on modelling and assessing the cost-competitiveness of organic PV technologies based on cost estimations for existing pilot-scale (kW-range), and projected scale-up (100MW) and industrial-scale (100GW) manufacturing capacity levels. Our generic results applying to all PV technologies show that PV systems installed at residential houses in Greece perform economically better than those in Denmark do in terms of self-sufficiency and gross electricity bill savings (i.e. excluding PV costs). Using the two country cases, which present very different settings, we characterise and discuss the influence of three key parameters of the economic performance of PV systems, namely the PV regulatory scheme, the solar irradiation level and the temporal match between the electricity consumption and solar irradiation profiles. Focusing on organic PV systems developed in an industrial-scale cost setting (1.53€/Wp), we find that they deliver significant electricity bill savings for residential houses in Greece (38%) under current conditions, while they may not be sufficiently attractive for residential houses in Denmark (6.5%) due to mainly the different PV regulatory schemes. Based on these findings, we therefore recommend investors interested in renewable energy technologies to pursue scaling up the manufacturing capacity of OPV technologies, as well as assess a large number of countries to identify and prioritise financially attractive settings for PV self-consumption.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Quantitative Sustainability Assessment, Department of Management Engineering, University of Western Macedonia
Authors: Chatzisideris, M. D. (Intern), Laurent, A. (Intern), Christoforidis, G. C. (Ekstern), Krebs, F. C. (Intern)
Pages: 471-479
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 208
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Coupling between creep and redox behavior in nickel - yttria stabilized zirconia observed in-situ by monochromatic neutron imaging

Ni-YSZ (nickel - yttria stabilized zirconia) is a material widely used for electrodes and supports in solid oxide electrochemical cells. The mechanical and electrochemical performance of these layers, and thus the whole cell, depends on their microstructure. During the initial operation of a cell, NiO is reduced to Ni. When this process is conducted under external load, like also present in a stack assembly, significant deformations of NiO/Ni-YSZ composite samples are
observed. The observed creep is orders of magnitude larger than the one observed after reduction during operation. This phenomenon is referred to as accelerated creep and is expected to have a significant influence on the microstructure development and stress field present in the Ni-YSZ in solid oxide electrochemical cells (SOCs), which is highly important for the durability of the SOC. In this work we present energy selective neutron imaging studies of the accelerated creep phenomenon in Ni/NiO-YSZ composite during reduction and also during oxidation. This approach allowed us to observe the phase transition and the creep behavior simultaneously in-situ under SOC operation-like conditions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, Proton conductors, Xnovo Technology ApS, Paul Scherrer Institut, European Spallation Source ESS AB
Authors: Makowska, M. G. (Intern), Kuhn, L. T. (Intern), Frandsen, H. L. (Intern), Lauridsen, E. M. (Ekstern), De Angelis, S. (Intern), Cleemann, L. N. (Intern), Morgano, M. (Ekstern), Trtik, P. (Ekstern), Strobl, M. (Ekstern)
Pages: 167-175
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 340
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.968 SNIP 1.726
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.597 SNIP 1.489
Web of Science (2007): Indexed yes
Cross-flow heat exchanger design using thermofluid topology optimization

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Haertel, J. H. K. (Intern), Engelbrecht, K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern)
Number of pages: 2
Publication date: 2017

Host publication information
Title of host publication: Proceedings of ICCHM^2T 2017
Article number: 160006
Main Research Area: Technical/natural sciences
Conference: 10th International Conference on Computational Heat, Mass and Momentum Transfer (ICCHM^2T 2017), Seoul, Korea, Democratic People's Republic of, 28/05/2017 - 28/05/2017
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Decisive Intermediates Responsible for the Carbonaceous Products of CO₂ Electro-reduction on Nitrogen-Doped sp² Nanocarbon Catalysts in NaHCO₃ Aqueous Electrolyte

Nitrogen-doped sp² nanocarbon materials have been considered promising catalysts for CO₂ electro-reduction. However, a fundamental understanding about product selectivity and the reaction routes is still lacking. In this report, the reaction mechanism on nitrogen-doped sp² nanocarbon materials is resolved by clarifying the authentic origin of the carbonaceous products: CO and HCO₂⁻. Two carbon-reduction pathways are identified based on a series of comparative studies by using differential electrochemical mass spectrometry and in situ CO adsorption experiments: a dominant pathway leading to CO from CO₂ and a secondary pathway leading to HCO₂⁻ from HCO₃⁻. Neither hydrocarbon (CₓHᵧ) nor alcohol or aldehyde (CₓHᵧOz) were detected in the reduction of CO₂. However, CO, which is generally regarded as an intermediate to be transformed into these products on metal catalysts, can undoubtedly be produced and adsorbed on nitrogen-doped sp² nanocarbon catalysts during the reaction.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Chinese Academy of Sciences, University of Messina
Authors: Xu, J. (Ekstern), Zhang, B. (Ekstern), Wang, B. (Ekstern), Wu, K. (Ekstern), Peng, Z. (Ekstern), Li, Q. (Intern), Centi, G. (Ekstern), Su, D. S. (Ekstern)
Number of pages: 5
Pages: 1274-1278
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemElectroChem
Design, enhanced Thermal and Flow efficiency of a 2KW active magnetic regenerator

The goal of the Danish ENOVHEAT project is to design and realize a high-efficiency magnetocaloric heat pump for the residential sector, based on the active magnetic regenerator (AMR) technology. Such a heat pump should have a coefficient of performance (COP) of at least 5, while giving a heating power of 1500 W over a temperature span of 25 K.

This paper explains several details of the device, such as the design of the magnet, the regenerator housing and the flow system. In particular, this paper investigates the best geometry for the regenerator bed to achieve a thermal and mechanically efficient housing to be used in the AMR system. Particular attention has been given to the reduction of the parasitic losses through the regenerator housing: both heat leaks between the magnetocaloric material (MCM) and an adjacent iron ring and the surroundings through a lid on top of the regenerator. These quantities have been decreased by creating an embossment on the bottom surface of the regenerator and by placing a thin rubber sheet between the magnetocaloric material and the steel lid, respectively.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Number of pages: 10
Publication date: 2017
Main Research Area: Technical/natural sciences
Magnetic refrigeration, Active magnetic regeneration, Regenerator housing geometry, Heat transfer
Source: PublicationPreSubmission
Source-ID: 137616391
Publication: Research - peer-review › Paper – Annual report year: 2017

Design of oxide electrocatalysts for efficient conversion of CO2 into liquid fuels

Electrochemical conversion of CO2 into high energy density liquid fuels utilizing renewable electricity can usher in a carbon neutral society without limiting the energy consumption. Lack of active and efficient electrocatalysts for this reaction remains a challenge. Research efforts towards catalyst development have obtained limited success due to adsorbate scaling relations on metallic surfaces. Preliminary experimental results indicate rutile oxide catalysts are active at very low overpotential, although the scientific understanding is missing. This thesis aims at delivering knowledge of atomic scale reaction thermodynamic needed to engineer efficient and active oxide electrocatalysts.

Rutile oxides are explored for CO2 reduction reaction (CO2RR) through density functional theory based simulation of reaction thermodynamics. Oxygen atom coordinated intermediates constitute the reaction mechanism active on such catalysts, annulling the scaling laws that limit metallic catalysts. Utilizing model rutile oxide surfaces, trends and limitations of CO2RR on oxide catalysts are analyzed. OH* binding energy is established as the descriptor for CO2RR activity on oxide surfaces. Scaling law based thermodynamic volcano relation for CO2RR is constructed. Guidelines for H*
and OH* binding energy range for good activity and selectivity of oxide CO2RR catalysts is proposed. This provides guidance to future development of oxide CO2RR catalysts.

The key role of CO* spectators on reaction onset potential and product selectivity of RuO2 electrocatalyst is elucidated through simulations of CO2RR pathway with varying CO* coverage level. The effect of adsorbate-adsorbate interaction in CO2RR activity is significant. Steric effects from spectator coverage also play a role by altering binding geometry of adsorbates. It is concluded that under experimental condition, CO* coverage is necessary for methanol evolution from RuO2 electrocatalyst, but very high coverage lead to evolution of formic acid and hydrogen together.

Building on the understanding of descriptors for CO2RR activity and CO* spectator effects, a new method of further enhancing the oxide electrocatalyst activity is proposed utilizing ligand effects in mixed oxide systems. Such effects in CO2RR catalysts can produce striking behaviours for adsorbate binding and catalytic properties. Detailed study of such properties for Ru/Ir mixed oxide surfaces with varying metal atom composition as well as different CO* coverages is done. It is identified that monolayer or lesser amount of iridium oxide on RuO2 catalyst can have a methanol onset potential of -0.2 V below RHE. This is attributed to a combination of ligand effect and adsorbate interaction. Through thermodynamic and kinetic barrier calculations, the possibility of 2C products is explored.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Bhowmik, A. (Intern), Vegge, T. (Intern), Hansen, H. A. (Intern)
Number of pages: 147
Publication date: 2017

**Publication information**

Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences

**Relations**

Projects:
Design of oxide electrocatalysts for efficient conversion of CO2 into liquid fuels
Source: PublicationPreSubmission
Source-ID: 139937932
Publication: Research › Ph.D. thesis – Annual report year: 2017

**Determination of the bonding strength in solid oxide fuel cells' interfaces by Schwickerath crack initiation test**

An adaptation of the Schwickerath crack initiation test (ISO 9693) was used to determine the bonding strength between an anode support and three different cathodes with a solid oxide fuel cell interconnect. Interfacial elemental characterization of the interfaces was carried out by SEM/EDS analysis on fracture surfaces to investigate the bonding mechanisms. SEM/EDS of fresh fractures were also performed to determine the cohesion/adhesion mechanism of bonding. Calculations of the residual stresses were determined by finite element simulation using ANSYS, based on thermo-mechanical properties of the materials obtained by measurement, calculation or literature.

**General information**

State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage, Brno University of Technology, Academy of Sciences of the Czech Republic, University of Modena and Reggio Emilia
Authors: Boccaccini, D. N. (Intern), Sevec, O. (Ekstern), Frandsen, H. L. (Intern), Dlouhy, I. (Ekstern), Molin, S. (Intern), Charlas, B. (Intern), Hjelm, J. (Intern), Cannio, M. (Ekstern), Hendriksen, P. V. (Intern)
Pages: 3565-3578
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 11
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Determination of the Resistance of Cone-Shaped Solid Electrodes

A cone-shaped electrode pressed into an electrolyte can with advantage be utilized to characterize the electro-catalytic properties of the electrode, because it is less dependent on the electrode microstructure than e.g. thin porous composite electrodes, and reactions with the electrolyte occurring during processing can be avoided. Newman's formula for current constriction in the electrolyte is then used to deduce the active contact area based on the ohmic resistance of the cell, and
from this the surface specific electro-catalytic activity. However, for electrode materials with low electrical conductivity (like Ce$_{1-x}$Pr$_x$O$_{2-\delta}$), the resistance of the cell is significantly influenced by the ohmic resistance of the cone electrode, wherefore it must be included. In this work the ohmic resistance of a cone is modelled analytically based on simplified geometries. The two analytical models only differ by a model specific pre-factor, which is consequently determined by a finite element model. The model was applied to measurements on cones of Ce$_{1-x}$Pr$_x$O$_{2-\delta}$ characterized on a YSZ electrolyte. Conclusively, the finite element model was used to obtain a formula for the resistance for different cone angles with a small contact area. This reproduces Newman’s formula for a cone angle equal to 90°, i.e. a semi-infinite body.
Development and Performance of Zirconia Based Oxygen Transport Membranes for Carbon Capture Processes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Pirou, S. (Intern), Hendriksen, P. V. (Intern), Kaiser, A. (Intern), Kiebach, W. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-5
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_119.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Development of Dual-Phase Oxygen Transport Membranes for Carbon Capture Processes

Fossil fuel based power plants and industrial production of cement and steel are major sources of anthropogenic CO2 emissions. One of the most promising approaches to capture and store CO2 from such large point sources is the oxy-fuel combustion route, where pure oxygen instead of air is used in the combustion, which greatly facilitates the down-stream CO2 capture. The main energy penalty for the oxy-fuel process is related to the production of the oxygen, which today commonly is done in cryogenic air separation units (ASUs). An alternative approach, which requires significant less energy is the use of oxygen transport membranes (OTMs), which has the potential to reduce the cost and energy penalty associated with the CO2 capture and storage.

This thesis focusses on the development and characterization of highly efficient and chemically stable planar asymmetric OTMs for direct integration in oxy-fuel combustion power plants. For the case of direct integration considered here the permeate side of the OTMs will be swept with recirculated flue gas whereby a driving force for oxygen transport through the membrane, which is fed with air on the other side, is directly established. It further facilitates thermal integration and thermal management in the combustion and avoids the need to handle pure oxygen. However, a direct integration scheme impose quite severe conditions on the membrane materials, such as stability towards both CO2 and SO2 and at low pO2 (1-10 mbar).

The development of planar asymmetric membranes in this work, required the parallel development of (i) stable porous supports, (ii) thin dense membrane layers, (iii) porous catalytic backbones and (iv) meso-porous nano-particulate catalytic coatings. For the dense membrane layers, dual-phase composites consisting of a stable ionic and a stable electronic conductor were used to overcome the stability limitations commonly observed with single-phase membrane materials (e.g. La1−xSrxCoyFe3O6 (LSCF), Ba1−xSrCo1−yFe3O6 (BSCF)) in CO2 and SO2. Three composite materials,
(ZrO2)0.89(Y2O3)0.01(Sc2O3)0.10 - MnCo2O4 (10Sc1YSZ-MCO), (ZrO2)0.89(Y2O3)0.01(Sc2O3)0.10 - Al0.02Zn0.98O1.01 (10Sc1YSZ-AZO) and (ZrO2)0.89(Y2O3)0.01(Sc2O3)0.10 - LaCr0.85Cu0.10Ni0.05O3-δ (10Sc1YSZ-LCCN) were prepared and applied in planar dual-phase asymmetric OTMs and finally characterized and tested in clean as well as flue-gas like atmospheres.

The work dedicated to 10Sc1YSZ-MCO (70-30 vol.%) dual-phase membranes entailed development and characterisation of 7 μm thin asymmetric membranes supported on zirconia supports as well as 0.5 mm thick self-standing membranes. The thin asymmetric membranes were prepared by tape-casting, lamination, and fired in a two-step sintering process in order to obtain fully dense thin membrane layers in a sintering regime that avoids excessive Co and Mn diffusion and/or decomposition of the MCO phase. Long-term stability tests over 1700 h in pure CO2 and 170 h in oxy-fuel conditions (250 ppm of SO2, 3 vol.% of H2O, 5 vol.% of O2 balanced with CO2) demonstrated the stability of the composite membranes under relevant application conditions. Oxygen permeation fluxes of 1.41 mLN cm-2 min-1 and 2.23 mLN cm-2 min-1 at 940 °C in air/N2 and O2/N2 atmospheres, respectively, were obtained. To further improve the membrane performance, catalytic surface layers were developed and tested by electrochemical impedance spectroscopy (EIS). Oxygen permeation tests were realized on 10Sc1YSZ-MCO (70-30 vol.%) membranes coated with these porous catalytic layers. The tests demonstrated that layers based on mixed ionic and electronic conducting backbones worked best (e.g. Ce0.8Tb0.2O2-δ (CTO)-NiFe2O4 (NFO) (40-60 vol.%)); increases in the oxygen permeation of about 50 % were observed for membranes coated with a such compared to those based on purely ionic conducting backbones.

10Sc1YSZ-AZO (50-50 vol.%) dual-phase composite membranes were also developed and characterized as thick (1 mm) self-standing membranes and thin (8 μm) supported membranes. The stability of these membranes in gas streams containing CO2, SO2 and H2O was found to be excellent. However, the high volatility of the Zn in the AZO phase under mildly reducing atmospheres makes the fabrication of thin asymmetric membranes challenging. Very limited oxygen permeation fluxes were measured through the 8 μm thick supported membrane (0.16 mLN cm-2 min-1 at 925 °C in air/N2), while 1 mm thick membranes, in which the Zn depleted part was removed by polishing, displayed higher oxygen permeation fluxes (0.33 mLN cm-2 min-1 at 925 °C in air/N2). Finally, self-supported dual-phase membranes made of 70 vol.% of 10Sc1YSZ and 30 vol.% of LCCN were prepared and characterized (oxygen permeation measurements and stability tests under oxy-fuel conditions). Analyses using several characterization techniques (X-ray diffraction (XRD), X-ray fluorescence (XRF), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy and scanning electronic microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) underlined the excellent stability of the materials under application relevant atmospheres. Oxygen permeation fluxes of 0.27 mLN cm-2 min-1 and 1.02 mLN cm-2 min-1 were obtained at 950 °C in air/N2 gradient for a 1000 μm thick and a 110 μm thick membrane, respectively. To further improve the oxygen permeation through 10Sc1YSZ-LCCN membranes, thin asymmetric and symmetric supported membranes were developed on 10Sc1YSZ-LCCN (40-60 vol.%) porous structures. Fully dense thin membrane layers (10-60 μm) were obtained, but the porous structures (support and activation layers) became too dense in the co-firing process. Consequently, further research and development is required to realize the full potential of this promising material combination.
stacks at high temperature and in controlled atmosphere. The methodology uses a mechanical loading rig designed to apply variable as well as constant loads on samples within a gas-tight high temperature furnace. In addition, a unique remotely installed length measuring setup involving laser micrometer is used to monitor deformations in the sample. Application of the methodology is exemplified by measurement of stress relaxation, creep and constant strain rate behaviors of a high temperature alloy used in the construction of SOC metallic interconnects at different temperatures. Furthermore, measurements using the proposed methodology are also verified with literature and experiments conducted using other machines.

**General information**
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Central Florida
Authors: Tadesse Molla, T. (Intern), Greco, F. (Ekstern), Kwok, K. (Ekstern), Zielke, P. (Intern), Frandsen, H. L. (Intern)
Number of pages: 21
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Testing and Evaluation
ISSN (Print): 0090-3973
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.63 SJR 0.354 SNIP 0.715
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.322 SNIP 0.453 CiteScore 0.44
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.29 SNIP 0.556 CiteScore 0.4
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.258 SNIP 0.428 CiteScore 0.35
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.281 SNIP 0.709 CiteScore 0.45
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.274 SNIP 0.676 CiteScore 0.44
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.307 SNIP 0.631
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.257 SNIP 0.555
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.309 SNIP 0.638
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.341 SNIP 0.597
Scopus rating (2006): SJR 0.278 SNIP 0.717
Scopus rating (2005): SJR 0.32 SNIP 0.718
Scopus rating (2004): SJR 0.473 SNIP 0.868
Scopus rating (2003): SJR 0.227 SNIP 0.55
Scopus rating (2002): SJR 0.499 SNIP 1.03
Scopus rating (2001): SJR 0.261 SNIP 0.673
Scopus rating (2000): SJR 0.619 SNIP 0.809
Scopus rating (1999): SJR 0.359 SNIP 0.787
Original language: English

**High temperature mechanical testing rig, Solid oxide fuel cells, Interconnects, Viscoplasticity**
Development of outdoor luminescence imaging for drone-based PV array inspection
This work has the goal to perform outdoor defect detection imaging that will be used in a fast, accurate and automatic drone-based survey system for PV power plants. The imaging development focuses on techniques that do not require electrical contact, permitting automatic drone inspections to be perform quicker and with less manpower. The final
inspection method will combine several techniques such as, infrared (IR), electroluminescence (EL), photoluminescence (PL), and visual imaging. Solar plant inspection in the future can be restricted only by imaging speed requirements, allowing an entire new perspective in large-scale PV inspection.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Organic Energy Materials, Department of Photonics Engineering, Diode Lasers and LED Systems, Coding and Visual Communication, Centre of Excellence for Silicon Photonics for Optical Communications, Skive Kommune, Kenergy, SiCon • Silicon and PV consulting, Aalborg University, Sky-Watch A/S


**Number of pages:** 2

**Publication date:** 2017

**Host publication information**

**Title of host publication:** Proceedings of the 44th IEEE Photovoltaic Specialists Conference, PVSC 2017

**Publisher:** IEEE

**Series:** Proceedings of the 44th IEEE Photovoltaic Specialists Conference, PVSC 2017

**Main Research Area:** Technical/natural sciences

**Conference:** 2017 IEEE Photovoltaic Specialists Conference, Washington D.C., United States, 25/06/2017 - 25/06/2017

**Relations**

**Projects:**

Development of outdoor luminescence imaging for drone-based PV array inspection

**Source:** FindIt

**Source-ID:** 2355411135

**Publication:** Research - peer-review › Article in proceedings – Annual report year: 2017

**Development of Robust Metal-Supported SOFCs and Stack Components in EU METSAPP Consortium**

The potential of MS-SOFCs was demonstrated through the previous EU METSOFC project, which concluded that the development of oxidation resistant novel metal-supported solid oxide fuel cell (MS-SOFC) design and stack is the requirement to advance this technology to the next level. The following EU METSAPP project has been executed with an overall aim of developing advanced metal-supported cells and stacks based on a robust, reliable and up-scalable technology. During the project, oxidation resistant nanostructured anodes based on modified SrTiO3 were developed and integrated into MS-SOFCs to enhance their robustness. In addition, the manufacturing of metal-supported cells with different geometries, scalability of the manufacturing process was demonstrated and more than 200 cells with an area of ~150 cm² were produced. The electrochemical performance of different cell generations was evaluated and best performance and stability combination was observed with doped SrTiO3 based anode designs. Furthermore, numerical models to understand the corrosion behavior of the MS-SOFCs were developed and validated. Finally, the cost effective concept of coated metal interconnects was developed, which resulted in 90% reduction in Cr evaporation, three times lower Cr2O3 scale thickness and increased lifetime. The possibility of assembling these cells into two radically different stack designs was demonstrated.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Mixed Conductors, Imaging and Structural Analysis, University of St Andrews, Karlsruhe Institute of Technology KIT, ICE Strömungsforschung GmbH, AVL List GmbH, Chalmers University of Technology, Sandvik Materials Technology AB, EiringKlinger AG


**Pages:** 508-516

**Publication date:** 2017

**Conference:** 12th European SOFC & SOE Forum, Lucerne, Switzerland, 05/07/2016 - 05/07/2016

**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Fuel Cells

**Volume:** 17
Direct Coal Oxidation in Modified Solid Oxide Fuel Cells

Hybrid direct carbon fuel cells employ a classical solid oxide fuel cell together with carbon dispersed in a carbonate melt on the anode side. In a European project, the utilization of various coals has been investigated with and without addition of an oxidation catalyst to the carbon-carbonate slurry or anode layer. The nature of the coal affects both open circuit voltage and power output. Highest OCV and power densities were observed for bituminous coal and by adding manganese oxide or praseodymium-doped ceria to the carbon/carbonate mixture. Comparing the carbon black fueled performance of an anode supported (315 μm anodes) and cathode supported cell (15 μm anode) indicates a superior performance of the latter. Using un-catalyzed biomass (charcoal) as fuel results in an OCV of 941 mV and a maximum power density of 78 mW/cm² at 755°C similar to the power output of manganese oxide catalyzed bituminous coal (73 mW/cm²).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Centro Nacional del Hidrogeno
Authors: Deleebeeck, L. (Intern), Gil, V. (Intern), Ippolito, D. (Intern), Campana, R. (Ekstern), Kammer Hansen, K. (Intern), Holtappels, P. (Intern)
Pages: F333-F337
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 4
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Discovery of high-performance low-cost n-type Mg3Sb2-based thermoelectric materials with multi-valley conduction bands

Widespread application of thermoelectric devices for waste heat recovery requires low-cost high-performance materials. The currently available n-type thermoelectric materials are limited either by their low efficiencies or by being based on expensive, scarce or toxic elements. Here we report a low-cost n-type material, Te-doped Mg3Sb1.5Bi0.5, that exhibits a very high figure of merit \(zT\) ranging from 0.56 to 1.65 at 300-725 K. Using combined theoretical prediction and experimental validation, we show that the high thermoelectric performance originates from the significantly enhanced power factor because of the multi-valley band behaviour dominated by a unique near-edge conduction band with a sixfold valley degeneracy. This makes Te-doped Mg3Sb1.5Bi0.5 a promising candidate for the low- and intermediate-temperature thermoelectric applications.
Dual phase composites for tubular oxygen transport membranes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Martinez Aguilera, L. (Intern), Bjørnetun Haugen, A. (Intern), Kiebach, W. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-18
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_128.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Dynamic and Impure Perovskite Structured Metal Oxide Surfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Hansen, K. V. (Intern), Norrman, K. (Intern), Traulsen, M. L. (Intern), Mogensen, M. B. (Intern)
Number of pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-02
Article number: 1724
ISSN (Print): 2151-2043
Original language: English
Links:
Dynamic and Impure Perovskite Structured Metal Oxide Surfaces

Surfaces of LSF and LSCF perovskite model electrodes were investigated using a variety of analytical methods on flat model electrodes that were prepared as either pellets or as thin films on top of YSZ pellets in order to throw more light on the widely discussed segregation of layers and particles on the electrode surfaces. An experimental test of the suggestion that the segregation might happen in the vacuum in the analysis equipment gave a negative result. Formation of particles containing significant amounts of S and Cr from segregation of the trace impurities in the acquired powders were observed, and lead us to a new hypothesis about the differences between flat model electrodes and technical nano-sized composite electrodes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Hansen, K. V. (Intern), Norrman, K. (Intern), Traulsen, M. L. (Intern), Mogensen, M. B. (Intern)
Pages: 91-100
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 80
Issue number: 9
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
Electronic versions:
Dynamic_and_Impure_Pеровскite_Structured_Metal_Oxide_Surfaces_IMCC_11_postprint.pdf
DOIs:
10.1149/08009.0091ecst
Publication: Research - peer-review › Conference article – Annual report year: 2017
Effect of CeO2 Addition on Hybrid Direct Carbon Fuel Cell Performance

The effect of CeO2 infiltration into the anode or CeO2 mixed with the carbon-fuel on the performance of a Hybrid Direct Carbon Fuel Cell (HDCFC) was studied through the use of polarization curves and electrochemical impedance spectroscopy. The use CeO2 in both ways helped to increase the cell performance. In particular, mixing CeO2 with carbon represents the best strategy to increase the cell power output, probably due to increased formation of CO.

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Ippolito, D. (Intern), Deleebeeck, L. (Intern), Kammer Hansen, K. (Intern)
Pages: F328-F332
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 4
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Effect of coating density on oxidation resistance and Cr vaporization from solid oxide fuel cell interconnects

- Protective action of dense and porous spinel coatings on Crofer 22 APU was compared.
- Reduction and re-oxidation produces denser coatings than heat treating in air only.
- Coating density has minor influence on oxidation resistance at 800 °C in air.
- Dense coating resulted in three times lower Cr evaporation rate than porous coating.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Chalmers University of Technology, Norwegian University of Science and Technology
Authors: Talic, B. (Intern), Falk-Windisch, H. (Ekstern), Venkatachalam, V. (Intern), Hendriksen, P. V. (Intern), Wiik, K. (Ekstern), Lein, H. L. (Ekstern)
Pages: 57-67
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 354
ISSN (Print): 0378-7753
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
- ISI indexed (2013): ISI indexed yes
Effect of Sr-doping of LaMnO$_3$ spacer on modulation-doped two-dimensional electron gases at oxide interfaces

Modulation-doped oxide two-dimensional electron gas formed at the LaMnO$_3$ (LMO) buffered disordered-LaAlO$_3$/SrTiO$_3$ (d-LAO/LMO/STO) heterointerface provides new opportunities for electronics as well as quantum physics. Herein, we studied the dependence of Sr-doping of La$_{1-x}$Sr$_x$MnO$_3$ (LSMO, $x=0$, 1/8, 1/3, 1/2, and 1) spacer on the transport properties of d-LAO/LSMO/STO in order to determine the effects of the filling of Mn $e_g$ subbands as well as the LSMO polarity on the modulation-doping. Upon increasing the LSMO film thickness from 1 unit cell (uc) to 2 uc, a sharp metal to insulator transition of interface conduction was observed, independent of $x$. The resultant electron mobility is higher than 1900 cm$^2$ V$^{-1}$ s$^{-1}$ at 2 K, which increases upon decreasing $x$. The sheet carrier density, on the other hand, is in the range of 6.9 $\times$ 10$^{12}$ to 1.8 $\times$ 10$^{13}$ cm$^{-2}$ (0.01 $\sim$ 0.03 e/uc) and is largely independent on $x$ for all the metallic d-LAO/LSMO (1 uc)/STO interfaces. These results are consistent with the charge transfer induced modulation doping scheme and clarify that the polarity of the buffer layer plays a trivial role on the modulation doping. The negligible tunability of the carrier density could result from the reduction of LSMO during the deposition of disordered LAO or that the energy levels of Mn 3$d$ electrons at the interface of LSMO/STO are hardly varied even when changing the LSMO composition from LMO to SrMnO$_3$.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Effects of Gold Substrates on the Intrinsic and Extrinsic Activity of High-Loading Nickel-Based Oxyhydroxide Oxygen Evolution Catalysts

We systematically investigate the effects of Au substrates on the oxygen evolution activities of cathodically electrodeposited nickel oxyhydroxide (NiOOH), nickel–iron oxyhydroxide (NiFeOOH), and nickel–cerium oxyhydroxide (NiCeOOH) at varying loadings from 0 to 2000 nmol of metal/cm². We determine that the geometric current densities, especially at higher loadings, were greatly enhanced on Au substrates: NiCeOOH/Au reached 10 mA/cm² at 259 mV overpotential, and NiFeOOH/Au achieved 140 mA/cm² at 300 mV overpotential, which were much greater than those of the analogous catalysts on graphitic carbon (GC) substrates. By performing a loading quantification using both inductively coupled plasma optical emission spectrometry and integration of the Ni²+/³⁺ redox peak, we show that the enhanced activity is predominantly caused by the stronger physical adhesion of catalysts on Au. Further characterizations using impedance spectroscopy and in situ X-ray absorption spectroscopy revealed that the catalysts on Au exhibited lower film resistances and higher number of electrochemically active metal sites. We attribute this enhanced activity to a more homogeneous electrodeposition on Au, yielding catalyst films with very high geometric current densities on flat substrates. By investigating the mass and site specific activities as a function of loading, we bridge the practical geometric activity to the fundamental intrinsic activity.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Energy Conversion and Storage, Stanford University, SLAC National Accelerator Laboratory
Authors: Chakthranont, P. (Ekstern), Kibsgaard, J. (Intern), Gallo, A. (Ekstern), Park, J. (Ekstern), Mitani, M. (Ekstern), Sokaras, D. (Ekstern), Kroll, T. (Ekstern), Sinclair, R. (Ekstern), Mogensen, M. B. (Intern), Jaramillo, T. F. (Ekstern)
Number of pages: 11
Pages: 5399-5409
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Catalysis
Volume: 7
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74
Web of Science (2014): Indexed yes
Efficient p-n junction-based thermoelectric generator that can operate at extreme temperature conditions

In many industrial processes a large proportion of energy is lost in the form of heat. Thermoelectric generators can convert this waste heat into electricity by means of the Seebeck effect. However, the use of thermoelectric generators in practical applications on an industrial scale is limited in part because electrical, thermal, and mechanical bonding contacts between the semiconductor materials and the metal electrodes in current designs are not capable of withstanding thermal-mechanical stress and alloying of the metal-semiconductor interface when exposed to the high temperatures occurring in many real-world applications. Here we demonstrate a concept for thermoelectric generators that can address this issue by replacing the metallization and electrode bonding on the hot side of the device by a p-n junction between the two semiconductor materials, making the device robust against temperature induced failure. In our proof-of-principle demonstration a p-n junction device made from nanocrystalline silicon is at least comparable in its efficiency and power output to conventional devices of the same material and fabrication process, but with the advantage of sustaining high hot side temperatures and oxidative atmosphere.
Electric Field-Assisted Pressureless Sintering of Ceramic Protonic Conductors

Gadolinium, yttrium and samarium-doped barium cerate pressed pellets were submitted to flash sintering experiments isothermally in the temperature range 800-1300°C under 200 V cm⁻¹ electric field. The pellets were positioned inside a dilatometer furnace with Pt-Ir electrodes connected either to a power supply or to an impedance analyzer to evaluate the bulk and the grain boundary contributions to the electrical resistivity. Near full density was achieved in the sintered samples. The combined results of dilatometry and impedance measurements in conventionally and flash sintered specimens show substantial improvement of the electrical conductivity. Joule heating is assumed to be the primary effect for sintering. Improved grain-to-grain contact and the removal of depleted chemical species due to Joule heating at the space charge region are proposed, respectively, as the reasons for the decrease of the grain boundary component in the
impedance diagrams and the improvement of the bulk electrical conductivity.

**Electric Field-Assisted Pressureless Sintering of Ceramic Protonic Conductors**

Gadolinium, yttrium and samarium-doped barium cerate (BCGd, BCY and BCSm, respectively) polycrystalline green pellets were submitted to electric field-assisted pressureless sintering experiments isothermally in the temperature range 800-1200°C under 100-200 V cm\(^{-1}\) electric fields, limiting to 1-5 A the electric current pulse amplitude. The sintering experiments were carried out in ambient atmosphere with the pellets positioned inside a vertical dilatometer furnace with Pt-Ir electrodes connected either to a power supply for applying the electric field or to an impedance analyzer for collecting \([-Z''(\omega) \times Z'(\omega)]\) data to evaluate the bulk and the grain boundary contributions to the electrical resistivity. Near full density was achieved in the sintered samples. The combined results of dilatometry and impedance spectroscopy measurements before and after flash sintering show substantial improvement of the electrical conductivity of flash sintered specimens. Joule heating is assumed to be the primary effect of the electric current pulse through the specimens.
Improved grain-to-grain contact and the removal of depleted chemical species due to Joule heating at the space charge region are proposed, respectively, as the reasons for the almost total disappearance of the grain boundary component in the impedance diagrams and the improvement of the bulk electrical conductivity.

Electrocatalysis caught in the act

Electrocatalytic conversion of biomass-derived chemicals in alkaline electrochemical cell

Electrochemical Characterization of a PEMEC Using Impedance Spectroscopy

In this study, electrochemical impedance spectroscopy (EIS) is applied in combination with cyclic voltammetry (CV) and current density – cell voltage curves (iV-curves) to investigate the processes contributing to the total impedance of a polymer electrolyte membrane electrolysis cell (PEMEC). iV-curves were linear above 0.35 A cm⁻² implying ohmic processes to be performance limiting, however the impedance spectra showed three arcs indicating three electrochemical reactions at these conditions not to be purely ohmic, but also to have capacitive properties. A hypothesis that the
composite IrOx/Nafion anode catalyst layer causes two of these arcs with a constant sum of resistance and current constrictions cause the third arc, is suggested. This hypothesis implies that the total differential cell resistance at current densities above 0.35 A cm\(^{-2}\) is purely ascribed to protonic resistance in Nafion in this type of PEMEC.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, EWII Fuel Cells A/S
Authors: Elsøe, K. (Intern), Grahl-Madsen, L. (Ekstern), Hjelm, J. (Intern), Scherer, G. (Ekstern), Hjelm, J. (Intern), Mogensen, M. B. (Intern)
Pages: F1419-F1426
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochemical Society. Journal
Volume: 164
Issue number: 13
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.611 SNIP 1.54
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.519 SNIP 1.484
Electrochemical Reduction of CO2 on Compositionally Variant Au-Pt Bimetallic Thin Films

The electrocatalytic reduction of CO2 on Au-Pt bimetallic catalysts with different compositions was evaluated, offering a platform for uncovering the correlation between the catalytic activity and the surface composition of bimetallic electrocatalysts. The Au-Pt alloy films were synthesized by a magnetron sputtering co-deposition technique with tunable composition. It was found that the syngas ratio (CO:H2) on the Au-Pt films is able to be tuned by systematically controlling the binary composition. This tunable catalytic selectivity is attributed to the variation of binding strength of COOH and CO intermediates, influenced by the surface electronic structure (d-band center energy) which is linked to the surface composition of the bimetallic films. Notably, a gradual shift of the d-band center away from the Fermi level was observed with increasing Au content, which correspondingly reduces the binding strength of the COOH and CO intermediates, leading to the distinct catalytic activity for the reduction of CO2 on the compositionally variant Au-Pt bimetallic films. In addition, the formation of formic acid in the bimetallic systems at reduced overpotentials and higher yield indicates that synergistic effects can facilitate reaction pathways for products that are not accessible with the individual components.
Electrochemical Reduction of CO$_2$ on Ir$_{x}$Ru$_{(1-x)}$O$_2$(110) Surfaces

High overpotentials and low faradic efficiencies plague metal catalysts for direct conversion of CO$_2$ to methanol and other liquid fuels. RuO$_2$-based electrocatalysts have been observed to evolve methanol at low overpotentials, which has been attributed to an alternative reaction mechanism with oxygen-coordinated intermediates that can circumvent the limitations imposed by the scaling relations on metal catalysts. Here, we introduce an innovative concept of ligand effects in oxide catalysts. Both IrO$_2$ and RuO$_2$ binds OH* and other intermediates from the electrochemical reduction of CO$_2$ (CO$_2$RR) strongly, but the stable and miscible system Ir$_x$Ru$_{(1-x)}$O$_2$ exhibits anomalous weaker binding energy in the presence of CO* spectators, because of Ru–Ir ligand effects. The weakened adsorbate binding leads to a very low CO$_2$RR onset potential (methanol evolution at −0.2 V RHE). An Ir atom at the bridge site with Ru neighbors binds intermediates such as OH* and OCHO* much weaker, because of synergistic ligand effects and adsorbate–adsorbate interactions. Consequently, a RuO$_2$ surface doped with Ir move close to the top of the predicted CO$_2$RR volcano for oxides, which offers a significant improvement over state-of-the-art electrocatalysts for conversion of CO$_2$ into methanol. Analysis of electronic structure parameters with adsorbate binding energies indicates the ligand effect depletes electrons from the Ir atom and shifts the t$_{2g}$ orbitals. The lack of electron donation from CO* spectators to Ir at the active site cause favorable adsorbate binding.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Bhowmik, A. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 8502–8513
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Catalysis
Volume: 7
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.271 SNIP 1.859 CiteScore 7.41
ISI indexed (2013): ISI indexed yes
Electrochemical Study of (La0.6Sr0.4)0.99CoO3-δ Thin Film Microelectrodes

Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC) are one of the most promising reversible energy conversion/storage technologies. Long term durability is required for such devices to become economically feasible. One approach to make SOCs more durable and at a lower cost is to decrease the operation temperature. However, lowering the operation temperature of SOCs has shown to be challenging due to the difficulty in finding suitable oxygen electrodes which have high catalytic activity for oxygen reduction and fast ionic transport. (La,Sr)CoO3-δ (LSC) is one of the promising cathode materials due to its high electronic and ionic conductivity as well as good catalytic activity for oxygen reduction at intermediate temperatures (500-700 °C). However, LSC is characterized by low chemical stability. Multiple degradation mechanisms are reported for LSC such as zirconate formation due to reactivity with YSZ (electrolyte) at operating temperature, decomposition at low pO2, SrO enrichment of and precipitation at the surface and Cr poisoning. Several studies on the electrochemical properties of oxygen electrode materials are reported in the literature. Most of the studies are performed on porous electrodes with the purpose of having a realistic scenario; however we still lack fundamental understanding of the underlying degradation mechanism. Even though porous electrode studies have provided invaluable information about the degradation of the oxygen electrode, the deconvolution of geometrical effects from the intrinsic properties of the material is very difficult. Therefore, the presented work aims to study the oxygen reduction mechanism using geometrically well-defined dense model electrodes. Gd doped CeO2 (CGO) was deposited on polished single crystals YSZ (100) and on top of the CGO layer was deposited a (La0.6Sr0.4)0.99CoO3-δ (LSC40) using pulsed laser deposition (PLD). The thin CGO film (~100 nm) was deposited to avoid any reaction between the YSZ and LSC40 (250 nm). Subsequently, using photolithography and ion beam etching the microelectrode arrays with varying diameters (from 100 µm to 5 µm) were produced. Each sample has 4 macro-electrodes which were used as counter-electrode while performing electrochemical measurements. To observe the effect of temperature on the film microstructure and chemistry one sample was heat treated for 16 hours. SEM images, AFM and ToF-SIMS reveal similar behavior for both heat treated and as-deposited films. ToF-SIMS depth profiling reveals a Sr and Co rich surface compared to the bulk of the LSC40 for both samples. The difference between the two samples are in the distribution of common impurities, such as silica. After the heat treatment, the Si signal is higher in the LSC/CGO and CGO/YSZ interfaces (See Figure 1 a-b)). The electrochemical measurements were recorded in a Controlled Atmosphere High Temperature Scanning Probe Microscope (CAHT-SPM)5which can reach temperatures up to 850 °C. The impedance spectra reveal a high frequency intercept which is related to the conductivity of the electrolyte, a small arc at high/middle frequencies originating from the electrode electrolyte interface, and finally a low frequency arc which is related to the air electrode interface. The evolution of the impedance spectra with changing temperature, atmosphere, polarization and microelectrode size combined with surface chemical analysis and imaging techniques reveals information about the underlying degradation mechanism of LSC electrodes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Chemistry
Authors: Kreka, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern), Norrman, K. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)
Publication date: 2017
Event: Abstract from 232nd ECS meeting, National Harbor, Washington, DC, United States.
Main Research Area: Technical/natural sciences
Source: FindIt
Source-ID: 2304160853
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Embedded plasmonic nanoparticles in high refractive index TiOx matrix for photovoltaics applications
Resume: More frequently high refractive index dielectric matrix are used in thin film photovoltaics as transporting layers with good optical properties. Doping such matrix with plasmonic resonant scatterers is a promising way to further increase
energy conversion efficiencies by trapping incoming light in ultrathin solar cells. Colloidal plasmonic oligomers are obtained following a cost-effective self-assembly strategy and incorporated in organic based cells produced using spincoating techniques in ambient air conditions. An interesting increase is observed of both external quantum efficiency (EQE) and short-circuit current for solar cells loaded with plasmonic oligomers compared with reference organic cells. Theoretical calculations demonstrate that the wavelength dependent EQE enhancement is a resonant process due to the increased scattering efficiency in plasmonic antennas allowed by a chemically controlled 1 nm nanogap. The nanogap antennas are linked at a controlled distance of a few nanometers by Dithiothreitol molecules. The spacing molecules ensure a minimum distance that plays a fundamental role in the formation of intensity hot spots in the nanogap as well as large and redshifted scattering peaks. This OPV device, realized in ambient air condition, exhibited an efficiency 14% higher than the reference one showing a relevant enhancement in the red part of the EQE measurements.

**Encapsulated iron-based oxygen reduction electrocatalysts by high pressure pyrolysis**

Non-precious metal catalysts (NPMCs) are candidate materials to replace platinum for proton exchange membrane fuel cells (PEMFCs). Herein we reported a type of iron-based NPMCs prepared by high pressure pyrolysis for the oxygen reduction reaction (ORR) in acidic media. The catalysts are in form of carbon microspheres in a sub-microscale consisting of iron-containing nanoparticles encapsulated by graphitic layers. By tailoring temperatures and duration of pyrolysis, the best ORR catalyst was achieved at 700 degrees C and 75 min, which exhibits an onset potential of 0.85 V at 0.1 mA cm(-2) and a half-wave potential of 0.72 V in acid media. After 10,000 potential cycles, only 25 mV shift of half-wave potential is observed showing excellent stability. An analogue material prepared from nitrogen-free precursors shows significant electrochemical activity though it is much lower than that from the nitrogen containing precursors and can be improved by post treatment in ammonia. These results indicate the contribution to the catalysis from surface nitrogen functionalities and encapsulated metal-containing nanoparticles. (C) 2017 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.
Energy modelling towards low carbon development of Beijing in 2030

Beijing, as the capital of China, is under the high pressure of climate change and pollution. The consumption of non-renewable energy is one of the most important sources of the CO2 emissions, which cause climate changes. This paper presents a study on the energy system modelling towards renewable energy and low carbon development for the city of Beijing. The analysis of energy system modelling is organized in two steps to explore the alternative renewable energy system in Beijing. Firstly, a reference energy system of Beijing is created based on the available data in 2014. The EnergyPLAN, an energy system analysis tool, is chosen to develop the reference energy model. Secondly, this reference model is used to investigate the alternative energy system for integrating renewable energies. Three scenarios are developed towards the energy system of Beijing in 2030, which are: (i) reference scenario 2030, (ii) BAU (business as usual) scenario 2030, and (iii) RES (renewable energies) scenario 2030. The 100% renewable energy system with zero
CO2 emission can be achieved by increasing solar energy, biomass and municipal solid waste (MSW) and optimizing heating system. The primary fuel consumption is reduced to 155.9 TWh in the RES scenario, which is 72 % of fuel consumption in the reference scenario 2030.
Energy supply modelling of a low-CO₂ emitting energy system: Case study of a Danish municipality

Municipal activities play an important role in national and global CO₂-emission reduction efforts, with Nordic countries at the forefront thanks to their energy planning tradition and high penetration of renewable energy sources. In this work, we present a case study of the Danish municipality of Sønderborg, whose aim is to reach zero net CO₂ emissions by 2029. Sønderborg has an official strategic plan towards 2029, which we compared with four alternative scenarios to investigate how the municipality could approach its target in the most energy-efficient and cost-effective way while simultaneously keeping biomass and waste consumption close to the limits of the locally available residual resources. We modelled all sectors of the energy system on the municipal scale, applying a broad range of energy conversion technologies, including advanced biomass conversion technologies and reversible electrolysis. We constructed five scenarios, each representing a different energy mix for Sønderborg’s energy system in 2029. We modelled these scenarios using the mixed-integer linear optimization tool Sifre. We compared the results for the five scenarios using four indicators: annual total system cost, total energy system efficiency, annual net system CO₂ emissions and total annual biomass consumption. The results show that scenarios with a high degree of electrification perform better on the selected indicators than scenarios with a high degree of biomass utilization. Moreover, the incorporation of advanced conversion technologies such as electrolysis, fuel cells and methanol production further reduces both the total system cost and net CO₂ of the highly electrified energy system. Our sensitivity analysis demonstrates that scenarios with a low biomass consumption and a high degree of electrification are less dependent on changes in energy prices. We conclude that in order to achieve their CO₂ emission goals in the most energy-efficient, cost-effective and sustainable way, municipalities similar to Sønderborg should compare a wide range of energy system configurations, for example, scenarios with a high degree of electrification and a limited biomass use.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Management Engineering, Systems Analysis, Energinet.dk
Authors: Sveinbjörnsson, D. Þ. (Intern), Ben Amer-Allam, S. (Intern), Hansen, A. B. (Ekstern), Algren, L. (Ekstern), Pedersen, A. S. (Intern)
Pages: 922-941
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 195
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Enhanced densification of thin tape cast Ceria-Gadolinium Oxide (CGO) layers by rheological optimization of slurries

Optimized CGO-based slurries are formulated and shaped into thin dense layers via a tape-casting process. The formulation is adjusted with respect to the rheological behaviour. The internal structure and flow properties of slurries are explored with the aim of identifying the required conditions to obtain thin dense CGO layers at reduced sintering temperatures (1200 °C). We demonstrate a correlation between the rheological properties of the slurries, the sintering behaviour and the microstructure of the resulting tapes. Remarkably, a dense CGO layer less than 20 μm thick is obtained with a non-congested slurry, having optimized ceramic loading and liquid-like behaviour.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors
Cerium-gadolinium oxide, Rheology, Thin dense layers, Tape casting, Sintering behaviour, Symmetric single-phase cells

DOIs:
10.1016/j.ceramint.2017.01.098
Environmental impacts of electricity self-consumption from organic photovoltaic battery systems at industrial facilities in Denmark

Organic photovoltaics (OPV) show promise of greatly improving the environmental and economic performance of PV compared to conventional silicon. Life cycle assessment studies have assessed the environmental impacts of OPV, but not under a self-consumption scheme for industrial facilities. We investigate the life cycle environmental impacts of electricity self-consumption from an OPV system coupled with a sodium/nickel chloride battery at an iron/metal industry in Denmark. Results show that an OPV system without storage could decrease the carbon footprint of the industry; installation of the battery increases climate change and human toxicity impacts. We discuss sensitive modelling parameters and provide recommendations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Quantitative Sustainability Assessment, Transport DTU, Department of Management Engineering
Authors: Chatzisideris, M. D. (Intern), Laurent, A. (Intern), Hauschild, M. Z. (Intern), Krebs, F. C. (Intern)
Pages: 45-48
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: C I R P Annals
Volume: 66
ISSN (Print): 0007-8506
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.93 SJR 1.672 SNIP 3.072
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.839 SNIP 3.185 CiteScore 3.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.73 SNIP 3.99 CiteScore 4.39
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.455 SNIP 3.875 CiteScore 3.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.175 SNIP 4.2 CiteScore 3.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.153 SNIP 3.507 CiteScore 2.81
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.172 SNIP 3.45
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.625 SNIP 2.205
Web of Science (2009): Indexed yes
Error Mitigation in Computational Design of Sustainable Energy Materials

Transportation based on sustainable energy requires an energy carrier, which is able to store the predominately electrical energy generated from sustainable sources in a high energy density form. Metal-air batteries, hydrogen and synthetic fuels are possible future energy carriers. Density functional theory calculations contribute in research and development of these technologies.

Systematic errors are present in calculations with general gradient approximation functionals for all three technologies. Such functionals will in many cases be the best compromise of computational cost and accuracy if not for the systematic errors. In this thesis it is shown how the systematic errors can be mitigated.

For different alkali and alkaline earth metal oxides, systematic errors have previously been observed. These errors are primarily caused by differences in metal element oxidation state. The systematic errors can be significantly reduced by using metal chlorides rather than pure bulk metals as point of reference for metal oxide energies.

Systematic errors in gas phase CO2 reduction reactions have previously been attributed a molecular O-C-O backbone structure. They are through error correlations found to be caused by individual C=O bonds. Energy corrections applied to C=O bonds significantly reduce systematic errors and can be extended to adsorbates.

A similar study is performed for intermediates in the oxygen evolution and oxygen reduction reactions. An identified systematic error on peroxide bonds is found to also be present in the OOH* adsorbate. However, the systematic error will almost be canceled by inclusion of van der Waals energy. The energy difference between key adsorbates is thus similar to that previously found.

Finally, a method is developed for error estimation in computationally inexpensive neural networks. The method can validate the use of a neural network for emulation of density functional theory calculations for given atomic configuration.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Christensen, R. (Intern), Vegge, T. (Intern), Hansen, H. A. (Intern)
Number of pages: 210
Publication date: 2017
Estimation of current constriction losses via 3D tomography reconstructions in electrochemical devices: a case study of a solid oxide cell electrode/electrolyte interface

In the present study, the methodology for accurate estimations of the current constriction resistance in solid state electrochemical devices via 3D tomography reconstructions is developed. The methodology is used to determine the current constriction resistances at the Ni:YSZ anode/YSZ electrolyte interface of a solid oxide fuel cell. The current constriction at this interface becomes increasingly important as thinner electrolyte layers are continuously being pursued for increased performance. Various possible scenarios have been illustrated on idealized geometries as a function of electrolyte thicknesses, from which it is clear, that for a given set of electrodes an optimal electrolyte thickness exist. Thus, increased performance by reduction of the electrolyte thickness is only feasible down to a certain thickness, after which, a lower performance is obtained on a further reduction of the electrolyte thickness. The obtained results on current constriction resistances from numerical calculations on a 3D reconstruction of a Ni:YSZ anode/YSZ electrolyte assembly is compared with existing models with analytical expressions. The comparison shows, that the assumptions of existing models are by far too simple and the models are therefore not applicable for technological relevant electrochemical devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis
Authors: Nielsen, J. (Intern), Jørgensen, P. S. (Intern)
Pages: 387-396
Publication date: 2017
Main Research Area: Technical/natural sciences
Interconnects used in Solid Oxide Cells stacks require protective coatings to lower their parabolic rate constant and block chromium evaporation (on the air side). In this work four different protective coatings on steel are evaluated for their high temperature corrosion resistance and electrical conductivity. A commercial electroplating process was used for the preparation of coatings with different Mn/Co ratios on Crofer 22 APU steel. Oxidation of samples was performed in air at 800°C for 1000 hours. Postmortem analysis of the coated samples was performed by scanning electron microscopy and x-ray diffractometry. Based on the results, influence of the Co/Mn ratio on the resulting corrosion properties are discussed. Parabolic rate constant of the coated samples is the lowest for the MnCo sample, whereas electrical resistance is the lowest for the Co sample, which has a corrosion rate similar to the not-coated alloys.

**Evaluation of electrodeposited Mn-Co protective coatings on Crofer 22 APU steel**

Interconnects used in Solid Oxide Cells stacks require protective coatings to lower their parabolic rate constant and block chromium evaporation (on the air side). In this work four different protective coatings on steel are evaluated for their high temperature corrosion resistance and electrical conductivity. A commercial electroplating process was used for the preparation of coatings with different Mn/Co ratios on Crofer 22 APU steel. Oxidation of samples was performed in air at 800°C for 1000 hours. Postmortem analysis of the coated samples was performed by scanning electron microscopy and x-ray diffractometry. Based on the results, influence of the Co/Mn ratio on the resulting corrosion properties are discussed. Parabolic rate constant of the coated samples is the lowest for the MnCo sample, whereas electrical resistance is the lowest for the Co sample, which has a corrosion rate similar to the not-coated alloys.

**General information**

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Molin, S. (Intern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences
Evolution of concentration fluctuation during phase separation of polystyrene/poly (vinyl methyl ether) blend in the presence of nanosilica

The influence of nanosilica on the concentration fluctuation of polystyrene/poly (vinyl methyl ether) (PS/PVME) mixtures was investigated during phase separation. The amplitude of concentration fluctuation was quantified by dielectric spectrums based on the idea of Lodge–Mcleish model and the linearized Cahn–Hilliard theory could describe the amplitude evolution of concentration fluctuation at the early stage of phase separation. Hydrophilic nanosilica A200 dispersed in PVME-rich phase behaved an obvious inhibition effect on the concentration fluctuation of blend matrix, while hydrophobic nanosilica R974 dispersed in PS-rich phase had little effect on the concentration fluctuation. The kinetics and amplitude evolution of concentration fluctuation during phase separation for PS/PVME/A200 nanocomposites were remarkably restrained due to the surface adsorption of PVME on A200. As the segmental dynamics of PVME and PS in homogeneous matrix was hardly influenced by A200 and R974, the enhanced miscibility and the significantly constrained flow relaxation of PVME chains might contribute to the retarded concentration fluctuation of PS/PVME/A200 nanocomposites. While the weak interaction between R974 and components of blend matrix and little effect of R974 on the molecular dynamics of PS chains may result in the weak retardation of concentration fluctuation for blend matrix.
Experimental and numerical comparison of multi-layered La(Fe, Si, Mn)_{13}H_y active magnetic regenerators

We present an experimental and numerical comparison of epoxy bonded multi-layered La(Fe, Si, Mn)_{13}H_y active magnetic regenerators. First, no-load tests were performed on four regenerators with two layers of material and varying amounts of epoxy (from 1 wt. % to 4 wt. %) in order to find the amount of epoxy necessary to maintain the mechanical integrity of the regenerators. As the second part of the study, experimental results of two regenerators with five and nine layers are compared to predictions from the one-dimensional numerical model. A maximum temperature span, $\Delta T_{\text{span}}$, over 20 K...
was measured and it is effectively equal for both regenerators. The numerical modelling was generally in good agreement with experimental results.

**General information**
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Iowa State University, Vacuumschmelze GmbH & Co. KG
Authors: Navickaité, K. (Intern), Bez, H. N. (Ekstern), Lei, T. (Intern), Barcza, A. (Ekstern), Vieyra, H. (Ekstern), Bahl, C. (Intern), Engelbrecht, K. (Intern)
Number of pages: 17
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: International Journal of Refrigeration
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.309 SNIP 1.737
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.841 SNIP 1.646
Scopus rating (2006): SJR 1.5 SNIP 1.629
Scopus rating (2005): SJR 1.409 SNIP 1.718
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.193 SNIP 1.933
Scopus rating (2003): SJR 1.241 SNIP 1.542
Experimental Determination of the Formation Enthalpy of Calcium Cobaltate from Sol–Gel Precursors

Calcium cobaltate (Ca₃Co₄O₉) remains one of the most promising p-type oxide materials for high-temperature thermoelectric energy conversion. While much progress has been made in refining our understanding of the unique structure of the material, as well as optimization of the transport properties for thermoelectric efficiency, there remains a gap in the knowledge, both experimental and theoretical, of the thermodynamics of the system. Presented herein is an analysis of the heat of formation of the Ca₃Co₄O₉ phase from sol–gel precursors using a highly sensitive differential scanning calorimeter, as well as observations of its decomposition into the Ca₃Co₂O₆ phase. The reaction enthalpy of forming Ca₃Co₄O₉ from CaCO₃ and Co₃O₄ sol–gel precursors was determined to be +284 (±2%) kJ/mol, leading to a standard enthalpy of Ca₃Co₄O₉ of −3307 (±3.5%) kJ/mol.

General information
State: Published
Authors: Holgate, T. C. (Ekstern), Wu, N. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern)
Number of pages: 5
Pages: 1413–1417
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Electronic Materials
Volume: 46
Issue number: 2
ISSN (Print): 0361-5235
Ratings:
  BFI (2018): BFI-level 1
  BFI (2017): BFI-level 1
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.586 SNIP 0.844 CiteScore 1.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.69 SNIP 1.083 CiteScore 1.82
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.713 SNIP 1.109 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.866 SNIP 1.318 CiteScore 1.74
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.841 SNIP 1.157 CiteScore 1.66
Ex-situ tracking solid oxide cell electrode microstructural evolution in a redox cycle by high resolution ptychographic nanotomography

For solid oxide fuel and electrolysis cells, precise tracking of 3D microstructural change in the electrodes during operation is considered critical to understand the complex relationship between electrode microstructure and performance. Here, for the first time, we report a significant step towards this aim by visualizing a complete redox cycle in a solid oxide cell (SOC) electrode. The experiment demonstrates synchrotron-based ptychography as a method of imaging SOC electrodes, providing an unprecedented combination of 3D image quality and spatial resolution among non-destructive imaging techniques. Spatially registered 3D reconstructions of the same location in the electrode clearly show the evolution of the microstructure from the pristine state to the oxidized state and to the reduced state. A complete mechanical destruction of the zirconia backbone is observed via grain boundary fracture, the nickel and pore networks undergo major reorganization and the formation of internal voids is observed in the nickel-oxide particles after the oxidation. These observations are discussed in terms of reaction kinetics, electrode mechanical stress and the consequences of redox cycling on electrode performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Paul Scherrer Institut
Authors: De Angelis, S. (Intern), Jørgensen, P. S. (Intern), Esposito, V. (Intern), Hsiao Rho Tsai, E. (Ekstern), Holler, M. (Ekstern), Kreka, K. (Intern), Abbeldahi, E. (Intern), Bowen, J. R. (Intern)
Pages: 520-527
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 360
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Fe-Ni Nanoparticles: A Multiscale First-Principles Study to Predict Geometry, Structure, and Catalytic Activity

Nanoparticles of iron and nickel are promising candidates as nanosized soft magnetic materials and as catalysts for carbon nanotube synthesis and CO methanation, among others. To understand geometry- and size-dependent properties of these nanoparticles, phase diagram of Fe/Ni alloy nanoparticles was calculated by density functional theory and cluster expansion method. Ground state convex is presented for FCC, BCC, and icosahedral particles. Previous experimental observations were explained by using multiscale model for particles with realistic size (diameter ≥ 2 nm). At size 1.5 nm,
geometry changes from BCC at low X(Ni) to icosahedral at high X(Ni). FCC is stabilized over icosahedral geometry by increasing number of atoms from 561 to 923. In large FCC particles, there is enrichment of Fe atoms from core to shell beneath surface, while surface and core are enriched by Ni atoms. Catalytic enhancement effect in CO methanation was found to be due to Ni incorporating in the active sites which brings adsorption energy of oxygen closer to the optimum. The predicted phase diagrams and implications on catalysis are expected to help rationalisation of experimental results and provide guidance for design of Fe/Ni-based nanomaterials.
Ferromagnetic Two-Dimensional Electron Gases at the Interface between Two Oxide Insulators

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences

From 3D to 2D Co and Ni Oxyhydroxide Catalysts: Elucidation of the Active Site and Influence of Doping on the Oxygen Evolution Activity

Layered oxyhydroxides (ox-hys) of Ni and Co are among the most active catalysts for oxygen evolution in alkaline media. Their activities can be further tuned by delamination into single-layer oxide sheets or by means of doping. The active site for the reaction and how doping and delamination promote the intrinsic activity, however, remain elusive. To shed light on these open questions, we have undertaken a systematic analysis of the stability, catalytic activity, and electronic conductivity of Ni and Co ox-hys ranging from bulk (3D) to single-layer (2D) catalysts. In both cases, we investigate the role of terrace and edge sites and use stability, catalytic activity, and electronic conductivity as evaluation criteria to pinpoint the best catalysts. We arrive at several important conclusions: the ox-hy surface is fully oxidized under oxygen evolution conditions, bulk terraces are ostensibly the most active sites, and Ni ox-hy sheets are more electronically conductive in comparison to their Co equivalents. Furthermore, we examine 25 different doped Co and Ni ox-hy nanosheets (V, Cr, Mn, Fe, CoNi, Cu, Ru, Rh, Pd, Ir, Pt, Ag, Al, Ga, In, Sn, Pb, Bi, Mg, Sc, Y, Ti, Nb, Zn, and Cd) to further tailor the catalytic performance. We establish the dependence of the electronic conductivity and activity on potential and find that it is more energetically favorable to dope Ni in comparison to Co ox-hys, with first-row transition and noble metals being the most stable dopants. Finally, we extend the analysis to include bulk terminations and reveal that most dopants, which are stable in the nanosheets, have a large propensity to segregate to the surface of bulk materials, and those that are less prone to segregation (Fe or Cr) are not electronically conductive in the bulk. Overall, we identify Rh-doped Ni ox-hy to be the best catalyst material.
Gel Electrolytes of Covalent Network Polybenzimidazole and Phosphoric Acid by Direct Casting

Polybenzimidazole membranes imbibed with phosphoric acid can support high proton conductivity at 120–200 °C, and have therefore emerged as the state-of-the-art electrolytes for fuel cells operating in this temperature range. This work presents a novel and operationally simple methodology for preparing mechanically robust covalent network polybenzimidazole membranes containing up to 95 wt% phosphoric acid. Diamino-terminal pre-polymers of different chain lengths are first prepared, followed by addition of a trifunctional carboxylic acid. The crude solutions are cast and subsequently heat treated at up to 230 °C, yielding free-standing membranes of networked polybenzimidazole with high proton conductivity at up to 180 °C and encouraging fuel cell performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Korea Institute of Science and Technology
Authors: Kirkebæk, A. (Intern), Aili, D. (Intern), Henkensmeier, D. (Ekstern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecular Materials and Engineering
Volume: 302
Issue number: 12
ISSN (Print): 1438-7492
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.894 SNIP 0.971
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Giant Electrostriction in highly defective oxides: The next generation of electromechanical materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science
Authors: Santucci, S. (Intern), Esposito, V. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-20
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_130.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Giant onsite electronic entropy enhances the performance of ceria for water splitting

Previous studies have shown that a large solid-state entropy of reduction increases the thermodynamic efficiency of metal oxides, such as ceria, for two-step thermochemical water splitting cycles. In this context, the configurational entropy arising from oxygen off-stoichiometry in the oxide, has been the focus of most previous work. Here we report a different source of entropy, the onsite electronic configurational entropy, arising from coupling between orbital and spin angular momenta in lanthanide f orbitals. We find that onsite electronic configurational entropy is sizable in all lanthanides, and reaches a maximum value of ≈4.7 k_B per oxygen vacancy for Ce^{4+}/Ce^{3+} reduction. This unique and large positive entropy source in ceria explains its excellent performance for high-temperature catalytic redox reactions such as water splitting. Our calculations also show that terbium dioxide has a high electronic entropy and thus could also be a potential candidate for solar thermochemical reactions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Northwestern University, Lawrence Livermore National Laboratory, Yale University
Authors: Naghavi, S. S. (Ekstern), Emery, A. A. (Ekstern), Hansen, H. A. (Intern), Zhou, F. (Ekstern), Ozolins, V. (Ekstern), Wolverton, C. (Ekstern)
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Communications
Volume: 8
Article number: 285
ISSN (Print): 2041-1723
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.399 SNIP 2.995
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.364 SNIP 3.053 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.331 SNIP 3.091 CiteScore 10.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.967 SNIP 2.776 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.586 SNIP 2.724 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.122 SNIP 1.544 CiteScore 4.44
ISI indexed (2011): ISI indexed no
Web of Science (2010): Indexed yes
Original language: English
Electronic versions:
s41467_017_00381_2.pdf
DOIs:
10.1038/s41467-017-00381-2
Source: PublicationPreSubmission
Source-ID: 134984169
Publication: Research - peer-review › Journal article – Annual report year: 2017
Giant tunability of the two-dimensional electron gas at the interface of γ-Al₂O₃/SrTiO₃

Two-dimensional electron gases (2DEGs) formed at the interface between two oxide insulators provide a rich platform for the next generation of electronic devices. However, their high carrier density makes it rather challenging to control the interface properties under a low electric field through a dielectric solid insulator, i.e. in the configuration of conventional field-effect transistors. To surpass this long-standing limit, we used ionic liquids as the dielectric layer for electrostatic gating of oxide interfaces in an electric double layer transistor (EDLT) configuration. Herein, we reported giant tunability of the physical properties of 2DEGs at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃ (GAO/STO). By modulating the carrier density thus the band filling with ionic-liquid gating, the system experiences a Lifshitz transition at a critical carrier density of 3.0×10¹³ cm⁻², where a remarkably strong enhancement of Rashba spin-orbit interaction and an emergence of Kondo effect at low temperatures are observed. Moreover, as the carrier concentration depletes with decreasing gating voltage, the electron mobility is enhanced by more than 6 times in magnitude, leading to the observation of clear quantum oscillations. The great tunability of GAO/STO interface by EDLT gating not only shows promise for design of oxide devices with on-demand properties, but also sheds new light on the electronic structure of 2DEG at the non-isostructural spinel/perovskite interface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Chemistry, Organic Chemistry, Technical University of Denmark, Nanjing University
Pages: 6878–6885
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Nano Letters
Volume: 17
Issue number: 11
ISSN (Print): 1530-6984
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 13.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
Glass transition of poly (methyl methacrylate) filled with nanosilica and core-shell structured silica

Core-shell (CS) nanocomposite particles with 53.4 wt% cross-linked poly (methyl methacrylate) (PMMA) shell of 11.6 nm in thickness were fabricated via miniemulsion polymerization of methyl methacrylate in the presence of modified nanosilica. The influence of nanosilica and CS nanoparticles on glass transition and segmental dynamics of PMMA in the nanocomposites prepared via solution casting was compared. The remarkable depression (≥10 °C) of glass transition temperature (T_g) induced by the incorporation of SiO_2 and CS was both observed at low loadings. Here, different mechanisms were responsible for the effect of SiO_2 and CS on the segmental acceleration of PMMA matrix. The formation of rigid amorphous fraction (RAF) layer around SiO_2 with the thickness of 16.4 nm led to the adjacent molecular packing frustration, while the “lubrication” effect of nonwetting interface between the grafted crosslinked chains and matrix chains resulted in the segmental acceleration and the reduction of dynamic fragility.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Zhejiang University
Authors: Song, Y. (Ekstern), Bu, J. (Ekstern), Zuo, M. (Ekstern), Gao, Y. (Ekstern), Zhang, W. (. (Intern), Zheng, Q. (Ekstern))
Pages: 141-149
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Polymer
Volume: 127
ISSN (Print): 0032-3861
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.77 SJR 1.191 SNIP 1.252
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.157 SNIP 1.286 CiteScore 3.72
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.321 SNIP 1.619 CiteScore 3.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.415 SNIP 1.666 CiteScore 4.07
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.591 SNIP 1.8 CiteScore 3.74
In the 1980s and 1990s, progress in fuel cell and battery research evolved mainly around materials development, empirical approaches, and efforts focusing mostly separately on either the microscale (electrodes and electrolytes) or the macroscale (systems, thermodynamics, and balance-of-plant). Since the 2000s, with the advent of more powerful computing and modeling resources, and the general progress in the field, it has seen a shift to the merging of scales, the possibility of 3D probing and quantification with fuel cell stacks and battery packs becoming the focal point. In parallel, disciplines have merged, too: a holistic and a detailed understanding in the range of underlying phenomena of chemistry, physics, materials science, and mechanical engineering has been combined with the addition of the influence of an electrical field or current. This union is essential to achieve the progress needed for the commercial breakthrough expected from the technologies. It became established that both experimental and modeling aspects deserve simultaneous and an equally weighted consideration, and it is recognized that the correspondences between models and experiments deliver among the most valuable advances to the field, due to the level of confidence and insight they provide.

**Guest Editorial**

In the 1980s and 1990s, progress in fuel cell and battery research evolved mainly around materials development, empirical approaches, and efforts focusing mostly separately on either the microscale (electrodes and electrolytes) or the macroscale (systems, thermodynamics, and balance-of-plant). Since the 2000s, with the advent of more powerful computing and modeling resources, and the general progress in the field, it has seen a shift to the merging of scales, the possibility of 3D probing and quantification with fuel cell stacks and battery packs becoming the focal point. In parallel, disciplines have merged, too: a holistic and a detailed understanding in the range of underlying phenomena of chemistry, physics, materials science, and mechanical engineering has been combined with the addition of the influence of an electrical field or current. This union is essential to achieve the progress needed for the commercial breakthrough expected from the technologies. It became established that both experimental and modeling aspects deserve simultaneous and an equally weighted consideration, and it is recognized that the correspondences between models and experiments deliver among the most valuable advances to the field, due to the level of confidence and insight they provide.

**General information**

State: Published


Authors: Van herle, J. (ed.) (Ekstern), Bowen, J. R. (ed.) (Intern)
High definition in-situ electro-optical characterization for Roll to Roll printed electronics

Resume: Printed electronics is emerging as a new, large scale and cost effective technology that will be disruptive in fields such as energy harvesting, consumer electronics and medical sensors. The performance of printed organic electronic devices relies principally on the carrier mobility and molecular packing of the polymer semiconductor material. Unfortunately, the analysis of such materials is generally performed with destructive techniques, which are hard to make compatible with in situ measurements, and pose a great obstacle for the mass production of printed electronics devices. A rapid, in situ, non-destructive and low-cost testing method is needed. In this study, we demonstrate that nonlinear optical microscopy is a promising technique to achieve this goal. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. We anticipate that this non-linear optical method will substantially contribute to the understanding of printed electronic devices and demonstrate it as a promising novel tool for non-destructive and facile testing of materials during printing of the device and at any moment during its lifespan. This will help the production and development of high quality printed technologies where the semiconductor material can be accessed by infrared light, such as solar cells, displays and sensors.
Highly Conformal Ni Micromesh as a Current Collecting Front Electrode for Reduced Cost Si Solar Cell

Despite relatively high manufacturing cost, crystalline-Si solar cell continues to hold promising future due to its high energy conversion efficiency and long life. As regards cost, one pertinent issue is the top electrode metallization of textured cell surface, which typically involves screen printing of silver paste. The associated disadvantages call for alternative methods that can lower the cost without compromising the solar cell efficiency. In the present work, a highly interconnected one-dimensional (1D) metal wire network has been employed as front electrode on conventional Si wafers. Here, for the first time, we report an innovative solution based crackle templating method for conformal metal wire network patterning over large textured surfaces. Laser beam induced current mapping showed uniform photocurrent collection by the electrodes without any shadow losses. With electroless deposition of Ni wire network on corrugated solar cell, a short circuit current of 33.28 mA/cm² was obtained in comparison to 20.53 mA/cm² without the network electrode. On comparing the efficiency with the conventional cells with screen printed electrodes, a 20% increment in efficiency has been observed. Importantly, the estimated manufacturing cost is at least two orders lower.

General information
State: Published
Authors: Gupta, N. (Ekstern), Rao, K. D. M. (Ekstern), Gupta, R. (Intern), Krebs, F. C. (Intern), Kulkarni, G. U. (Ekstern)
Pages: 8634-8640
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 9
Issue number: 10
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
High Mobility Two-dimensional Electron Gases at Complex Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 17
Publication date: 2017

Host publication information
Title of host publication: Metal Oxide-Based Thin Film Structures
Publisher: Elsevier Science
Edition: 1
ISBN (Print): 9780128111666
Chapter: 9
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 133867946
Publication: Research › Book chapter – Annual report year: 2017

High performance \(\text{LaNi}_{1-x}\text{Co}_x\text{O}_{3-\delta}\) (\(x = 0.4\) to \(0.7\)) infiltrated oxygen electrodes for reversible solid oxide cells

Oxygen electrodes prepared by infiltration of yttria stabilized zirconia backbone with \(\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{1.95}\) barrier layer and \(\text{LaNi}_{1-x}\text{Co}_x\text{O}_{3-\delta}\) (\(x = 0.4\) to \(0.7\)) catalyst for application in reversible solid oxide cells have been studied. The effect of temperature and Ni:Co ratio on their phase composition, microstructure and electrochemical properties are discussed. It was shown that oxygen electrodes infiltrated with \(\text{LaNi}_{0.6}\text{Co}_{0.4}\text{O}_{3-\delta}\) had the lowest polarization resistance, i.e. 67 mΩ cm\(^2\) at 600 °C. The performance of a fuel electrode supported solid oxide cell with infiltrated oxygen electrode in both fuel cell and electrolysis mode was tested. Electrochemical characterization of the solid oxide cell showed that the resistance contribution from these oxygen electrodes to the overall cell resistance is minor i.e. approximately 20 mΩ cm\(^2\) at a temperature of 700 °C. The cell was also tested in the steam electrolysis mode at a constant current of \(-1.0\) A cm\(^{-2}\) at 800 °C for 240 h. The oxygen electrode showed reasonable degradation rate with the oxygen electrode resistance of 33 mΩ cm\(^2\) at 700 °C after 240 h of testing.
How covalence breaks adsorption-energy scaling relations and solvation restores them

It is known that breaking the scaling relations between the adsorption energies of *O, *OH, and *OOH is paramount in catalyzing more efficiently the reduction of O2 in fuel cells and its evolution in electrolyzers. Taking metalloporphyrins as a case study, we evaluate here the adsorption energies of those adsorbates on the metal centers Cr, Mn, Fe, Co, Ni and Cu, using H, F, OH, NH2, CH3, and BH2 as ring ligands. We show that covalence systematically breaks scaling relations under vacuum by strengthening certain M-OOH bonds. However, covalence modifies adsorbate solvation in solution depending on the degree of covalence of the metal-adsorbate bonds. The two effects have similar magnitudes and opposite signs, such that scaling relations are restored in solution. Thus, solvation is a crucial ingredient that must be taken into account in studies aimed at breaking scaling relations in solution. Our findings suggest that the choice of metal and ligand determines the catalytic activity within the limits imposed by scaling relations, whereas the choice of an appropriate solvent can drive such activity beyond those limits.
Hydrogen Decrepitation Press-Less Process Recycling of NdFeB sintered magnets

A Hydrogen Decrepitation Press-Less Process (HD-PLP) recycling method for recycling of anisotropic NdFeB magnets is demonstrated. The method combines hydrogen decrepitation (HD) disintegration of the initial magnet, powder sieving and the Press-Less Process (PLP), where hydride powder is sintered in a graphite mold. Coercivities up to 534 kA/m were obtained in porous samples based on powder size $d < 100 \mu m$. Adding a ball milling step resulted in full density isotropic magnets for $d > 100 \mu m$. The coercivity reached $H_{ci} = 957$ kA/m being 86 % of the original N48M material without addition of rare earth elements.

General information
State: Published
Authors: Xia, M. (Intern), Abrahamsen, A. B. (Intern), Bahl, C. (Intern), Veluri, B. (Ekstern), Søegaard, A. I. (Ekstern), Bøjse, P. (Ekstern)
Pages: 55-61
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 441
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285 CiteScore 1.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.861 SNIP 0.897
In situ electrical and thermal monitoring of printed electronics by two-photon mapping

Printed electronics is emerging as a new, large scale and cost effective technology that will be disruptive in fields such as energy harvesting, consumer electronics and medical sensors. The performance of printed electronic devices relies principally on the carrier mobility and molecular packing of the polymer semiconductor material. Unfortunately, the analysis of such materials is generally performed with destructive techniques, which are hard to make compatible with in situ measurements, and pose a great obstacle for the mass production of printed electronics devices. A rapid, in situ, non-destructive and low-cost testing method is needed. In this study, we demonstrate that nonlinear optical microscopy is a promising technique to achieve this goal. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence and second harmonic response. We show that, in our experimental conditions, it is possible to relate the total amount of photoluminescence detected to important material properties such as the charge carrier density and the molecular packing of the printed polymer material, all with a spatial resolution of 400 nm. Importantly, this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, ICFO - Institute of Photonic Sciences
Authors: Pastorelli, F. (Intern), Accanto, N. (Ekstern), Jørgensen, M. (Intern), van Hulst, N. F. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 7
Article number: 3787
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Impact of Prosumers and their Clusters on the Energy System

General information
State: Published
Organisations: Department of Civil Engineering, Section for Building Energy, Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities
Authors: Larma, M. (Intern), Heller, A. (Intern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at Fourth General CITIES Consortium Meeting, Aarhus, Denmark.
Main Research Area: Technical/natural sciences

Improved performance of LaNi$_{0.6}$Fe$_{0.4}$O$_3$ solid oxide fuel cell cathode by application of a thin interface cathode functional layer

In this work, novel functional layers were prepared by a low temperature spray pyrolysis method on the oxygen side of the solid oxide cells. Thin layers of Ce$_{0.8}$Gd$_{0.2}$O$_2$ and LaNi$_{0.6}$Fe$_{0.4}$O$_3$ are prepared between the electrolyte and the porous oxygen electrode. Additionally, the influence of the sprayed ceria barrier layer on the zirconia based electrolyte with the new layers is evaluated. Impedance spectroscopy results show improvement in contact between the electrolyte and the porous cathode electrode. Additionally, electrochemical performance of the cathode is improved, as evidenced by a lowered area specific resistance and increased power density obtained from an anode supported cell employing the new layer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Molin, S. (Intern), Jasinski, P. Z. (Ekstern)
Number of pages: 4
Pages: 252-255
Publication date: 2017
Improving, characterizing and predicting the lifetime of organic photovoltaics: Topical Review

This review summarizes the recent progress in the stability and lifetime of organic photovoltaics (OPVs). In particular, recently proposed solutions to failure mechanisms in different layers of the device stack are discussed comprising both structural and chemical modifications. Upscaling is additionally discussed from the perspective of stability presenting the challenges associated with device packaging and edge protection. An important part of device stability studies is the characterization, and this review provides a short overview of the most advanced techniques for stability characterization reported recently. Lifetime testing and determination is another challenge in the field of organic solar cells and the final sections of this review discuss the testing protocols as well as the generic marker for device lifetime and the methodology for comparing all the lifetime landmarks in one common diagram. These tools were used to determine the baselines for OPV lifetime tested under different ageing conditions. Finally, the current status of lifetime for organic solar cells is presented and predictions are made for progress in the near future.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Pages: 1-35
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 50
Issue number: 10
Article number: 103001
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.645 SNIP 0.917
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.693 SNIP 1.046 CiteScore 2.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.069 SNIP 1.383 CiteScore 2.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.18 SNIP 1.469 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.244 SNIP 1.394 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.257 SNIP 1.399 CiteScore 2.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.291 SNIP 1.288
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.283 SNIP 1.337
Indoor measurement of angle resolved light absorption by antireflective glass in solar panels

In this work, we present measurements of angle resolved light absorption of antireflective (AR) glass of PV samples, performed indoors using a collimated high radiance broadband light source. This indoor method proved to be viable and offered a significant simplification compared to outdoor measurements with trackers. The experimental results showed optical responses that are stable and suitable for indoor characterization of solar cells. We find the characteristic optical response of six different antireflective glasses, and based on such measurements, we perform PVsyst simulations and present the monthly DC energy production estimates across four distinct latitudinal locations with six different glass types. The results indicated that the AR glasses present different optical effects at the angles intervals between 0 – 45° and 60 – 90° and that the Diffuse AR glass can improve monthly yields by as much as 2% relatively to a bare cell.

General information

State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Department of Micro- and Nanotechnology, Experimental Surface and Nanomaterials Physics
Number of pages: 4
Publication date: 2017

Host publication information
Title of host publication: Proceeedings of the 33rd European Photovoltaic Solar Energy Conference and Exhibition
Publisher: IEEE
Main Research Area: Technical/natural sciences
Antireflective glass, Angle of Incidence, Incidence Angle Modifier, Simulation
Electronic versions: Poster
Indoor Measurement of Angle Resolved Light Absorption by Black Silicon

Angle resolved optical spectroscopy of photovoltaic (PV) samples gives crucial information on PV panels under realistic working conditions. Here, we introduce measurements of angle resolved light absorption by PV cells, performed indoors using a collimated high radiance broadband light source. Our indoor method offers a significant simplification as compared to measurements by solar trackers. As a proof-of-concept demonstration, we show characterization of black silicon solar cells. The experimental results showed stable and reliable optical responses that makes our setup suitable for indoor, angle resolved characterization of solar cells.
Solid oxide fuel cell, Metal support, Lanthanum doped strontium titanate, Redox tolerance, Perovskite A site deficiency

Electronic versions:
1_s2.0_S0378775317314106_main.pdf

DOIs:
10.1016/j.jpowsour.2017.10.066

Source: FindIt
Source-ID: 2392778861

Publication: Research - peer-review › Journal article – Annual report year: 2017
Influence of carbon monoxide on the cathode in high-temperature polymer electrolyte membrane fuel cells

This paper describes the results of adding small amounts of CO gas to the cathode side in a HT-PEM fuel cell with a polybenzimidazole (PBI) membrane running on either oxygen or air. Experimental conditions: Temperature ranges 120–160 °C, constant current either 200 mA/cm² or 800 mA/cm² and CO ranges 0.1–1.3%. In this case it was found that small amounts of CO under special conditions have a beneficial effect on the potential of the fuel cells, whereas larger amounts can bring the potential down to almost zero. An interesting phenomenon is that after the flow of CO is switched off a temporary improvement of the potential is seen before the situation goes back to normal. A good explanation for this is a competition between CO, O₂ and H₃PO₄ at the three phase boundaries, also that a steady state exist in which CO constantly is oxidized to CO₂.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Søndergaard, S. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Bjerrum, N. J. (Intern)
Pages: 3309-3315
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication Information
Volume: 42
Issue number: 5
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.142 SNIP 1.286
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.294 SNIP 1.319 CiteScore 3.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.212 SNIP 1.494 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.278 SNIP 1.467 CiteScore 3.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.515 SNIP 1.729 CiteScore 3.96
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.456 SNIP 1.837 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.589 SNIP 1.871
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.333 SNIP 1.885
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.401 SNIP 2.096
The aim of this work is to assess the influence of a magnetic sample on the applied magnetic field inside the air gap of a magnetic circuit. Different magnetic sources including an electromagnet, a permanent magnet in a soft ferromagnetic toroidal yoke, as well as 2D and 3D Halbach cylinders are considered, using a numerical model. Gadolinium is chosen as magnetic material for the sample, due to its strong magnetocaloric properties and its wide use in magnetic refrigeration prototypes. We find that using uniform theoretical demagnetizing factors for cylinders or spheres results in a deviation of less than 2% in the calculation of internal magnetic fields at temperatures above the Curie point of gadolinium. Below the Curie point, a stronger magnetization of the cylinders and spheres leads to a larger deviation which can reach 8% when using uniform demagnetizing factors for internal magnetic field calculations.
Influence of porosity on mechanical properties of tetragonal stabilized zirconia

3YSZ specimens with variable open porosity (1–57%) were fabricated, and the stiffness, strength and fracture properties (fracture toughness and R-curve) were measured to investigate their potential use as support structures for solid oxide fuel or electrolysis cells. The ball-on-ring test was used to characterize Young's modulus and Weibull strength. The variation of fracture toughness with porosity was investigated and modelled using the results from fracture mechanical testing. A distinct R-curve behaviour was observed in dense 3YSZ specimens, in samples with a porosity around 15% and in some of the highly porous samples (porosities ~45%) reflecting a transformation toughening in the material. For the most porous samples, the “R-curve behaviour” disappeared and subcritical crack growth was observed. The studies indicate that even...
highly porous 3YSZ structures (porosities exceeding 40%) are feasible supports for SOFC/SOECs from a mechanical point of view.

**General information**

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Università degli Studi di Modena e Reggio Emilia
Authors: Boccaccini, D. (Intern), Frandsen, H. L. (Intern), Soprani, S. (Intern), Cannio, M. (Ekstern), Klemensø, T. (Intern), Gil, V. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 16
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: European Ceramic Society. Journal
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.392 SNIP 1.945
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.381 SNIP 1.724
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.146 SNIP 1.645
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.22 SNIP 1.76
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.191 SNIP 1.67
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.084 SNIP 1.637
Web of Science (2005): Indexed yes
Influence of Substrate-Film Reactions on YBCO Grown by Fluorine-Free MOD Route

Recently, fluorine-free metal organic deposition routes (FF-MOD) for growth of YBCO superconducting films have attracted increased attentions. In this paper, a comparison study was performed on the YBCO-Ag superconducting thin films deposited on two types substrates, LaAlO₃ and CSD-Ce₀.₉La₀.₁O₂₋ₓ (CLO)/YSZ, respectively. Although conventional TFA-MOD derived YBCO films exhibit high performance on both substrates, the results vary when using the FF-MOD precursor. SEM and XRD results reveal that c-axis and a/b-axis orientations coexist in the YBCO-Ag films grown on the CSD-CLO/YSZ substrate deposited by the FF-MOD route, while the BaCeO₃ by-product is a dominating phase in the fully reacted film. Based on the structural analysis of the partially converted films, we found that interfacial reactions between the film and the CLO cap layer play an essential role on the epitaxial growth of YBCO-Ag films from the FF-MOD solution. Because of the different chemical reaction path compared to conventional TFA-MOD routes, it seems that the polycrystalline BaCeO₃ formation takes place prior to the YBCO-Ag epitaxial growth associated with the melting process, which results in structural deterioration at high growth temperatures and, therefore, no superconductivity. This study indicates the necessity of further reducing the nucleation temperature of YBCO films processed by FF-MOD routes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Shanghai Jiao Tong University
Authors: Zhao, Y. (Ekstern), Tang, X. (Intern), Wu, W. (Ekstern), Grivel, J. (Intern)
Number of pages: 4
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication Information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 27
Issue number: 4
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.431 SNIP 1.171 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.575 SNIP 1.27 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
In-line, roll-to-roll morphology analysis of organic solar cell active layers

We present the first comparative in situ small and wide angle X-ray scattering study of two polymers that are relevant for organic photovoltaics, during coating on a flexible substrate. From the obtained measurements we identified several differences between the drying of the two polymers. The polymer optimized for roll-to-roll coating attained its final morphological packing nearly instantly after deposition, and had the shortest drying profile. We therefore conclude that fast-drying polymers which are influenced less by drying temperature or substrate inhomogeneities are better suited for roll-to-roll coating, and that fundamentally, the kinetics of drying dominate the process in the case of roll-to-roll slot-die coating.

General information
State: Published
Pages: 2411-2419
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: November
Issue number: 11
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
In operando Raman spectroscopy for investigation of solid oxide electrolysis cells

Summary. How can in operando Raman spectroscopy increase our understanding of degradation and activation processes in solid oxide electrolysis cells? Recent experimental results are reported, including experiments showing remarkable polarisation induced compositional changes in infiltrated perovskite electrodes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Montana State University
Authors: Traulsen, M. L. (Intern), Walker, R. A. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Pages: 167
Publication date: 2017

Host publication information
Title of host publication: 1st International Conference on Electrolysis - Book of abstracts
Main Research Area: Technical/natural sciences
Conference: Copenhagen, Denmark, 12/06/2017 - 12/06/2017
Electronic versions:
ICE2017_Traulsen_Marie_abstract.pdf
Links:
http://www.ice2017.net/Conference
Source: PublicationPreSubmission
Source-ID: 138261362
Publication: Research - peer-review → Conference abstract in proceedings – Annual report year: 2017
In Operando Raman spectroscopy for investigation of solid oxide electrolysis cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Montana State University
Authors: Traulsen, M. L. (Intern), Walker, R. A. (Ekstern), Hotlappels, P. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at International Conference on Electrolysis, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
2017_ICE_conference_poster_matr_.pdf
Publication: Research › Poster – Annual report year: 2017

In operando study of high-performance thermoelectric materials for power generation: a case study of β-Zn₄Sb₃

To bring current thermoelectric (TE) materials achievement into a device for power generation, a full understanding of their dynamic behavior under operating conditions is needed. Here, an in operando study is conducted on the high-performance TE material β-Zn₄Sb₃ under large temperature gradient and thermal cycling via a new approach using in situ transmission electron microscopy combined with characterization of the TE properties. It is found that after 30 thermal cycles in a low-pressure helium atmosphere the TE performance of β-Zn₄Sb₃ is maintained with the figure of merit, $zT$, value of 1.4 at 718 K. Under a temperature gradient of 380 K (Thot = 673 K and Tcold = 293 K) operating for only 30 h, zinc whiskers gradually precipitate on the cold side of the β-Zn₄Sb₃ leg. The dynamical evolution of Zn in the matrix of β-Zn₄Sb₃ is found to be the source that leads to a high $zT$ value by lowering of the thermal conductivity and electrical resistivity, but it is also the failure mechanism for the leg under these conditions. The in operando study brings deep insight into the dynamic behavior of nanostructured TE materials for tailoring future TE materials and devices with higher efficiency and longer durability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Ceramic Engineering & Science, TEGnology ApS, Aarhus University
Authors: Le, T. H. (Intern), Ngo, D. (Intern), Han, L. (Intern), Iversen, B. B. (Ekstern), Yin, H. (Ekstern), Pryds, N. (Intern), Van Nong, N. (Intern)
Number of pages: 17
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Electronic Materials
Volume: 3
Issue number: 10
Article number: 1700223
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.98 SJR 1.096 SNIP 0.567
Original language: English
DOIs:
10.1002/aelm.201700223
Source: PublicationPreSubmission
Source-ID: 134385036
Publication: Research - peer-review › Journal article – Annual report year: 2017

Inside or Outside? Linking Outdoor and Indoor Lifetime Tests of ITO-Free Organic Photovoltaic Devices for Greenhouse Applications

We present results from an installation of fully roll-to-roll printed and coated polymer solar cell modules in a greenhouse environment over the course of roughly 2 years (650 days). We explored two different device architectures based on either fully carbon-based electrodes or silver nanowire (AgNW)-based electrodes and two different barrier materials. We followed the ISOS protocols while studying the devices in three different greenhouse conditions in the Netherlands and compared to reference devices mounted outdoors in Denmark tested according to ISOS-O-1 and ISOS-O-2. We studied each condition and type in multiples to obtain acceptable statistics and found that the AgNW-based devices performed best in terms of stability.

General information
State: Published
In-situ formed Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$ barrier layers on yttria stabilized zirconia backbones by infiltration - A promising path to high performing oxygen electrodes of solid oxide cell

Oxygen electrodes for solid oxide cells were prepared by a consecutive infiltration of a gadolinium doped ceria (Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$, CGO) barrier layer and a lanthanum cobalt nickelate (La$_{0.96}$Co$_{0.4}$Ni$_{0.6}$O$_3$, LCN) electro catalyst layer into a porous yttrium doped zirconia (YSZ) backbone. The influences of the following parameters on the microstructure of the formed CGO barrier layer and on the electrochemical performance of the cells were studied: i) surfactants and wetting agents, ii) ceria/gadolinia coverage, iii) calcination profiles and iv) exposure temperature during testing. The infiltration process of the CGO barrier layer was optimized and a slow, pH controlled decomposition of urea containing precursor solutions was found to be most effective. For these cells a decrease of 84% in the polarization resistance ($R_p$) was achieved compared to cells without a barrier layer. Furthermore, a better initial performance and only a small increase of the cell-resistance with increasing exposure temperatures during testing were obtained. A complete and homogenous covering of the YSZ backbone with Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$ was found to be necessary to maintain high performance also at higher exposure temperatures (> 800 °C).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Pages: 51-59
Publication date: 2017
Main Research Area: Technical/natural sciences
In situ TEM analysis of a symmetric solid oxide cell in oxygen and vacuum–cation diffusion observations

In order to establish the use of solid oxide fuel/electrolysis cells (SOFC/SOEC) in the energy market, a deeper understanding of degradation effects during operation is necessary. This study applies in situ transmission electron microscopy (TEM) of a symmetric model cell composed by two oxygen electrodes of La$_0.6$Sr$_{0.4}$CoO$_{3-δ}$ (LSC) and an electrolyte, ZrO$_2$: 8% mol Y$_2$O$_3$ (8YSZ), deposited on 1% Nb doped SrTiO$_{3-δ}$ (STN) single crystal substrate by pulsed
laser deposition. The results showed a high cation mobility of the electrodes when exposed to 900 °C. Cobalt is found to agglomerate at the interface between LSC and STN. Strontium depletion is observed in both electrodes. Finally, a faster grain growth occurs in LSC for the cell exposed to oxygen in comparison with the cell in vacuum.

In-situ TEM studies of nanostructured thermoelectric materials: An application to Mg-doped Zn4Sb3 alloy
We demonstrate an advanced approach using advanced in-situ transmission electron microscopy (TEM) to understand the interplay between nanostructures and thermoelectric (TE) properties of high-performance Mg-doped Zn4Sb3 TE system. With the technique, microstructure and crystal evolutions of TE material have been dynamically captured as a function of temperature from 300 K to 573 K. On heating, we have observed clearly precipitation and growth of a Zn-rich secondary phase as nanoinclusions in the matrix of primary Zn4Sb3 phase. Elemental mapping by STEM-EDX spectroscopy reveals enrichment of Zn in the secondary Zn6Sb5 nanoinclusions during the thermal processing without decomposition observed. Such nanostructure strongly enhances the phonon scattering resulting in the decrease in the
thermal conductivity leading to a $zT$ value of 1.4 at 718 K.

**General information**

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science, University of Manchester
Authors: Ngo, D. (Intern), Le, H. T. (Intern), Ngo, N. V. (Intern)
Number of pages: 23
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Chemphyschem
ISSN (Print): 1439-4235
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.81 SJR 1.264 SNIP 0.771
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.334 SNIP 0.912 CiteScore 3.21
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.362 SNIP 0.905 CiteScore 3.12
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.442 SNIP 0.948 CiteScore 3.22
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.763 SNIP 0.955 CiteScore 3.24
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.719 SNIP 1.05 CiteScore 3.37
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.872 SNIP 1.031
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.91 SNIP 1.12
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 2.153 SNIP 1.098
- Scopus rating (2007): SJR 2.215 SNIP 1.129
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 2.008 SNIP 1.159
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 2.067 SNIP 1.147
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.799 SNIP 1.087
- Scopus rating (2003): SJR 1.666 SNIP 1.128
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 1.026 SNIP 0.79
In situ TEM study of the coarsening of carbon black supported Pt nanoparticles in hydrogen

The control of sizes and shapes of nanostructures is of tremendous importance for the catalytic activity in electrochemistry and in catalysis more generally. However, due to relatively large surface free energies, nanostructures often sinter to form coarser and more stable structures that may not have the intended physicochemical properties.

Pt is known to be a very active catalyst in several chemical reactions and for example as carbon supported nanoparticles in fuel cells.

The presentation focusses on coarsening mechanisms of Pt nanoparticles supported on carbon black during exposure to hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H₂/Ar while ramping up the temperature to ca. 900 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in the pure hydrogen environment are stable during constant temperature ramping by 10°C/min up to ca. 800 °C. The coarsening above this temperature is fully dominated by the particle migration and coalescence mechanism. This is contrary to supported Pt nanoparticles in oxygen, where the coarsening is fully dominated by Ostwald ripening. For agglomerated Pt nanoparticles, coalescence events were observed already at ca. 200 °C. The temperature-dependency of particle sizes and the observed migration distances are consistent with simple early models for the migration and coalescence.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Proton conductors, Huaihai Institution of Technology
Authors: Simonsen, S. B. (Intern), Wang, Y. (Ekstern), Jensen, J. O. (Intern), Zhang, W. (. (Intern)
Number of pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-02
Article number: 1433
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
2017_Simonsen_ECS_232th_meeting.pdf
Links:
http://ma.ecsdl.org/content/MA2017-02/32/1433.abstract?sid=7d22f381-06cc-4cd6-ab50-980f863bd550
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2017

In Situ Transmission Electron Microscopy in Materials Science - Possibilities and Prospects

General information
State: Published
Organisations: Center for Electron Nanoscopy, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Wagner, J. B. (Intern), Zhang, L. (Intern), Gualandris, F. (Intern), Simonsen, S. B. (Intern), Kuhn, L. T. (Intern), Beleggia, M. (Intern), Hansen, T. W. (Intern)
Number of pages: 3
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
Untitled.pdf
Integration of district cooling in smart energy systems: the case of Singapore

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, University of Zagreb, Aalborg University, Nanyang Technological University
Authors: Dominkovic, D. F. (Intern), Dobravec, V. (Ekstern), Bačeković, I. (Ekstern), Krajačić, G. (Ekstern), Romagnoli, A. (Ekstern)
Number of pages: 1
Publication date: 2017

Host publication information
Main Research Area: Technical/natural sciences

Relations
Projects:
Integration of district cooling in smart energy systems: the case of Singapore
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Intrinsic Conductivity in Magnesium-Oxygen Battery Discharge Products: MgO and MgO2
Nonaqueous magnesium–oxygen (or “Mg-air”) batteries are attractive next generation energy storage devices due to their high theoretical energy densities, projected low cost, and potential for rechargeability. Prior experiments identified magnesium oxide, MgO, and magnesium peroxide, MgO2, as the primary discharge products in a Mg/O2cell. Charge transport within these nominally insulating compounds is expected to limit battery performance; nevertheless, these transport mechanisms either are incompletely understood (in MgO2) or remain a matter of debate (in MgO). The present study characterizes the equilibrium conductivity associated with intrinsic (point) defects within both compounds using first-principles calculations. For MgO, negative Mg vacancies and hole polarons—the latter localized on oxygen anions—were identified as the dominant charge carriers. However, the large formation energies associated with these carriers suggest low equilibrium concentrations. A large asymmetry in the carrier mobility is predicted: hole polarons are highly mobile at room temperature, while Mg vacancies are essentially immobile. Accounting for nonequilibrium effects such as frozen-in defects, the calculated conductivity data for MgO is shown to be in remarkable agreement with the three “Arrhenius branches” observed in experiments, thus clarifying the long-debated transport mechanisms within these regimes. In the case of MgO2, electronic charge carriers alone—electron and hole polarons—are the most prevalent. Similar to MgO, the equilibrium concentration of carriers in MgO2 is low, and moderate-to-poor mobility further limits conductivity. If equilibrium behavior is realized, then we conclude that (i) sluggish charge transport in MgO or MgO2 will limit battery performance when these compounds cover the cathode support and (ii) what little conductivity exists in these phases is primarily electronic in nature (i.e., polaron hopping). Artificially increasing the carrier concentration via monovalent substitutions is suggested as a strategy for overcoming transport limitations.

General information
State: Published
Organisations: Atomic scale modelling and materials, Department of Energy Conversion and Storage, University of Michigan, DENSO International America
Authors: Smith, J. G. (Ekstern), Naruse, J. (Ekstern), Hiramatsu, H. (Ekstern), Siegel, D. J. (Intern)
Pages: 3152-3163
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry of Materials
Volume: 29
Issue number: 7
ISSN (Print): 0897-4756
Ratings:
BFI (2018): BFI-level 2
Investigating phase behavior and structural changes in NiO/Ni-YSZ composite with monochromatic in-situ 2D and static 3D neutron imaging

In this work, we report neutron imaging studies of redox cycling of NiO/Ni-8YSZ (nickel/nickel oxide – yttria stabilized zirconia) composite used for electrodes in solid oxide electrochemical cells for efficient energy conversion (power-to-gas and vice versa) purposes (i.e. for anodes in solid oxide fuel cells, and for cathodes in solid oxide electrolysis cells). Results of in-situ 2D and ex-situ 3D measurements are presented. In-situ observation of phase transition between NiO and Ni were performed at the test Beamline for neutron Optics and other Applications (BOA) at the continuous neutron source SINQ of Paul Scherrer Institut (PSI, Switzerland) by means of monochromatic neutron imaging, and post mortem monochromatic neutron tomography was performed at Helmholtz Zentrum Berlin (HZB) at the BER II reactor using the CONRAD-2 imaging instrument. Combining both time resolved radiography and post mortem tomography provides complementary information about the reduction/oxidation degree and e.g. crack evolution in the investigated system and it is therefore possible to acquire information about the rate of chemical reactions and spatial evolution of phases and morphological features.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, University of Bayreuth, Paul Scherrer Institut, Helmholtz–Zentrum Berlin für Materialien und Energie, Xnovo Technology ApS
Authors: Makowska, M. G. (Ekstern), Strobl, M. (Ekstern), Kardjilov, N. (Ekstern), Frandsen, H. L. (Intern), Manke, I. (Ekstern), Morgano, M. (Ekstern), Lacatusu, M. (Intern), De Angelis, S. (Intern), Lauridsen, E. M. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 5
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica B: Condensed Matter
ISSN (Print): 0921-4526
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.39 SJR 0.455 SNIP 0.848
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.488 SNIP 0.849 CiteScore 1.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.553 SNIP 0.942 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.555 SNIP 0.998 CiteScore 1.41
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.583 SNIP 0.888 CiteScore 1.21
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.586 SNIP 0.809 CiteScore 1.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.582 SNIP 0.707
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.594 SNIP 0.707
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.582 SNIP 0.646
Scopus rating (2007): SJR 0.551 SNIP 0.619
Investigation of a Spinel-forming Cu-Mn Foam as an Oxygen Electrode Contact Material in a Solid Oxide Cell Single Repeating Unit

A critical issue in state-of-the-art solid oxide cell stacks is the contacting of the oxygen electrode. The commonly used ceramic contact layers are applied in a green state and cannot be sintered properly, due to compliance limitations arising from other stack components like sealing glasses and steels. The consequence is a low layer and interface strength. A metallic copper manganese foam, which is oxidized under operation conditions into a conductive $\text{Cu}_{1+x}\text{Mn}_{2-x}\text{O}_4$ spinel, is presented in this work as a viable contact solution. The foam has been electrochemically tested in a single repeating unit setup for 350 hours of constant operation, followed by dynamic conditions with thermal cycles. After operation, a micro structural analysis using scanning electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction was carried out. It was confirmed that after oxidation/operation the manganese solely formed a $\text{CuMn}$-spinel phase, mixed with a $\text{CuO}$ phase. A separate Mn-oxide phase was not found. The conductivity and contacting of the foam was sufficient for > 350 h of SOFC operation. With an initial serial resistance comparable to single cell tests using gold foil as contact material and moderate degradation rates, the CuMn foam presented itself as an interesting cathode contact solution.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Applied Electrochemistry
Authors: Zielke, P. (Intern), Wulff, A. C. (Intern), Sun, X. (Intern), Jensen, S. H. (Intern), Frandsen, H. L. (Intern), Norby, P. (Intern), Hagen, A. (Intern)
Pages: 730-734
Publication date: 2017

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 5
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.699 SNIP 0.787 CiteScore 2.02
Investigation of Cu$_2$ZnSnS$_4$ nanoparticles for thin-film solar cell applications

We study the effect of the annealing atmosphere on grain growth of ligand-free and ligand-coated Cu$_2$ZnSnS$_4$ (CZTS) nanoparticle-based thin films by thermal analysis. We use thermogravimetric analysis (TGA) coupled with mass spectrometry (MS) to simultaneously monitor mass changes and evolved gases of both nanoparticle powders and inks. The investigation focuses on annealing in air, nitrogen, and forming gas (5% H$_2$ in Ar), i.e., oxidizing, inert, and reducing atmospheres. We find that the oleylamine capping ligands thermally decompose into smaller organic fragments starting below its boiling point, with a slightly higher decomposition rate in reducing atmosphere. With nanoparticle inks, very modest grain growth is observed, with no differences between the atmospheres. Conversely, with nanoparticle powders, micron-sized grains appear all over for the ligand-free sample and some micron-sized grains are seen with inert atmosphere for the ligand-coated powder. The starting material is thus very important for grain growth.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Mixed Conductors, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Agersted, K. (Ekstern), Crovetto, A. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Ion-Exchange-Induced Selective Etching for the Synthesis of Amino-Functionalized Hollow Mesoporous Silica for Elevated-High-Temperature Fuel Cells

As differentiated from conventional synthetic processes, amino-functionalized hollow mesoporous silica (NH2–HMS) has been synthesized using a new and facile strategy of ion-exchange-induced selective etching of amino-functionalized mesoporous silica (NH2-meso-silica) by an alkaline solution. Nuclear magnetic resonance (NMR) spectroscopy and in situ time-resolved small-angle X-ray scattering (SAXS) reveal that ion-exchange-induced selective etching arises from the gradient distribution of OH− in the NH2-meso-silica nanospheres. Moreover, the ion-exchange-induced selective etching mechanism is verified through a successful synthesis of hollow mesoporous silica. After infiltration with phosphotungstic acid (PWA), PWA–NH2–HMS nanoparticles are dispersed in the poly(ether sulfone)–polyvinylpyrroldione (PES–PVP) matrix, forming a hybrid PWA–NH2–HMS/PES–PVP nanocomposite membrane. The resultant nanocomposite membrane with an optimum loading of 10 wt % of PWA–NH2–HMS showed an enhanced proton conductivity of 0.175 S cm−1 and peak power density of 420 mW cm−2 at 180 °C under anhydrous conditions. Excellent durability of the hybrid composite membrane fuel cell has been demonstrated at 200 °C. The results of this study demonstrated the potential of the facile synthetic strategy in the fabrication of NH2–HMS with controlled mesoporous structure for application in nanocomposite membranes as a technology platform for elevated-temperature proton exchange membrane fuel cells.
Ionic/Electronic Conductivity, Thermal/Chemical Expansion and Oxygen Permeation in Pr and Gd Co-Doped Ceria Pr$_x$Gd$_{0.1}$Ce$_{0.9-x}$O$_{1.95-\delta}$

The oxygen permeation flux of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-\delta}$ (CGO)-based oxygen transport membranes under oxidizing conditions is limited by the electronic conductivity of the material. This work aims to enhance the bulk ambipolar conductivity of CGO by partial substitution of Ce with the redox active element Pr. A series of compositions of Pr$_x$Gd$_{0.1}$Ce$_{0.9-x}$O$_{1.95-\delta}$ ($x = 0, 0.02, 0.05, 0.08, 0.15, 0.25, 0.3$ and $0.4$) was prepared by solid state reaction. X-ray powder diffraction (XPD) indicates that Pr is completely dissolved in the fluorite structure up to 40 at.%. Pronounced nonlinear thermal expansion behavior was observed as a function of temperature, due to the simultaneous contributions of both thermal and chemical expansion. The electronic and ionic conductivities were measured as a function of temperature and oxygen partial pressure. Within the range from 10 to 15 at.% Pr, a drastic drop of the activation energy of the hole mobility and an abrupt increase of the hole conductivity at low temperature was observed. The behavior could be rationalized by a simple percolation model. Oxygen permeation fluxes through disk shaped samples fed with air on one side and N$_2$ on the other side were also measured. The oxygen flux through Pr$_{0.05}$Gd$_{0.1}$Ce$_{0.85}$O$_{1.95-\delta}$ was higher than that for CGO by one order of magnitude owing to the enhanced electronic conductivity albeit the flux is still limited by the electronic conductivity. In terms of the electronic and ionic conductivity, the estimated maximum oxygen permeation flux of a 10 μm Pr$_{0.4}$Gd$_{0.1}$Ce$_{0.5}$O$_{1.95-\delta}$-based membrane exceeds 10 Nml cm$^{-2}$ min$^{-1}$ at 900°C under a small oxygen potential gradient (0.21/10$^{-3}$ bar) which is promising for use in oxygen production and in oxy-fuel combustion. Also the material may be well applicable to SOFC/SOEC composite electrodes where mixed conductivity is also desirable.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Cheng, S. (Intern), Chatzichristodoulou, C. (Intern), Søgaard, M. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Pages: F1354-F1367
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Is γ-Al₂O₃ polar?

Polarity in thin films and polar discontinuities across an interface plays an important role in determining electronic properties. A key example is the conductivity at the LaAlO₃/SrTiO₃ (LAO/STO) interface, which is proposed to originate from the polarity of LAO. As a consequence, the conductivity does not disappear when LAO/STO is subjected to highly oxidizing conditions. Substituting LAO with another nominally polar material γ-Al₂O₃ (GAO) results in an interface conductivity which can be destroyed by annealing in oxygen. We investigate this apparent paradox by revisiting the defect spinel atomic structure of GAO. We show that the polarity is dependent on the distribution of aluminum vacancies which are intrinsically present in GAO to ensure charge neutrality. In particular, certain film thicknesses allow for vacancy distributions that make GAO nominally non-polar along the [001] direction. We further propose that electromigration of aluminum vacancies across atomic layers can alter the polarity, making the GAO film effectively act as a ferroelectric.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Authors: Christensen, D. V. (Intern), Smith, A. (Intern)
Number of pages: 4
Pages: 887-890
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Surface Science
Volume: 423
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.951 SNIP 1.225
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.914 SNIP 1.3 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.958 SNIP 1.477 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.965 SNIP 1.488 CiteScore 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.918 SNIP 1.373 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.908 SNIP 1.402 CiteScore 2.27
ISI indexed (2011): ISI indexed yes
Jahn-Teller and Non-Jahn-Teller Systems Involving CuF$_6^{4-}$ Units: Role of the Internal Electric Field in Ba$_2$ZnF$_6$:Cu$^{2+}$ and Other Insulating Systems

The applicability of the Jahn-Teller (JT) framework to 6-fold coordinated d$^9$ ions whose local symmetry is not strictly octahedral is explored by means of first principle calculations. Our results contradict much of the existing literature where these systems are analyzed within the quasi-JT regime which assumes the usual JT description with a small splitting between $b_{1g}$ ($\sim x^2-y^2$) and $a_{1g}$ ($\sim 3z^2-r^2$) orbitals and also the existence of three nearly equivalent distortions. To clarify this issue we investigate the equilibrium geometry (equatorial, $R_{eq}$, and axial, $R_{ax}$, Cu$^{2+}$-F$^-$ distances) and optical transitions for CuF$_6^{4-}$ units formed in Cu$^{2+}$-doped the tetragonal Ba$_2$ZnF$_6$ host lattice. While the experimental d-d transitions cannot be reproduced through the isolated CuF$_6^{4-}$ unit at the equilibrium geometry, a reasonable agreement is reached adding in the calculation the internal electric field, $E_R(r)$, created by the rest of lattice ions on the electrons confined in the complex. It is shown that this tetragonal field, $E_R(r)$, already produces a gap $\Delta_0 \sim 0.35$ eV between $b_{1g}$ ($\sim x^2-y^2$) and $a_{1g}$ ($\sim 3z^2-r^2$) orbitals of Ba$_2$ZnF$_6$:Cu$^{2+}$ when $R_{ax} = R_{eq}$. Nevertheless, as this internal field leads to a $\Delta_0$ value higher than typical JT barriers it drastically modifies the characteristic pattern of a JT effect. In particular, it prevents the existence of three equivalent distortions as confirmed by experimental EPR data. Furthermore, $E_R(r)$ is shown to be the main physical reason behind an unusual compressed ground state with the hole in the $a_{1g}$ ($\sim 3z^2-r^2$) level while it is always placed in the $b_{1g}$ ($\sim x^2-y^2$) level for MX$_6^-$ complexes ($M = Cu^{2+}, Ag^{2+}, Ni^{++}; X = F^-, Cl^-$) in cubic lattices displaying a static JT effect. While the experimental results of CuF$_6^{4-}$ in Ba$_2$ZnF$_6$ cannot be understood within the JT framework it is pointed out that a quasi-JT situation can however happen for a d$^9$ ion in a cubic lattice under a strain of $\sim 10^{-3}$ in agreement with experimental data. The present results stress the key role played by the internal electric fields for a quantitative understanding of compounds with transition metal cations. Moreover, they also demonstrate that in the interpretation of experimental data the use of a simple model should be avoided unless all its assumptions are well justified.

General information
State: Published
Organisations: Atomic scale modelling and materials, Theoretical Atomic-scale Physics, Universidad de Cantabria
Authors: Aramburu, J. A. (Ekstern), Garcia-Fernandez, P. (Ekstern), García Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Joining of Half-Heusler and Bismuth Tellurides for Segmented Thermoelectric Generators

Segmented generators where the p- or n-type legs are formed by joining materials in series enables each material to operate in their most efficient temperature range. Here, we have fabricated and characterized segmented thermoelectric p- and n-type legs based on bismuth tellurides and half-Heusler alloys p-type Hf0.5Zr0.5CoSn0.2Sb0.8 and n-type Ti0.6Hf0.4NiSn. A two-step process was introduced to join the half-Heusler to the bismuth tellurides to form a segmented structure which was then characterized for its thermoelectric and structural properties. The output power generation was characterized under various hot side temperatures up to 873 K with the cold side fixed at 323 K. The stability of the joints was also investigated under heat treatment and thermal cycling. Under working temperatures from 323 K to 873 K, the obtained p-type segmented legs could deliver a power density of 0.3 W cm\(^{-2}\) and maximum voltage of 115 mV. With the same condition, the power density and the maximum voltage generated by n-type segmented leg were 0.25 W cm\(^{-2}\) and 102 mV. The area-specific contact resistances of the p- and n-type legs were 50 \(\mu\Omega\) cm\(^{-2}\) and 35 \(\mu\Omega\) cm\(^{-2}\), respectively. The output performance of each leg was \(\sim 95\%\) after 6 cycles from 323 K to 873 K.

General information

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials
Authors: Ngan, P. H. (Intern), Han, L. (Intern), Christensen, D. V. (Intern)
Number of pages: 10
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Electronic Materials
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.586 SNIP 0.844 CiteScore 1.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.69 SNIP 1.083 CiteScore 1.82
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.713 SNIP 1.109 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.866 SNIP 1.318 CiteScore 1.74
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.841 SNIP 1.157 CiteScore 1.66
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.777 SNIP 1.049
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.927 SNIP 1.148
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.875 SNIP 0.961
Large Differences in the Optical Spectrum Associated with the Same Complex: The Effect of the Anisotropy of the Embedding Lattice

Transition-metal complexes with a well-defined geometry are usually considered to display almost the same properties independently of the system where they are embedded. Here we show that the above statement is not true depending on the anisotropy of the host lattice, which is revealed in the form of the electric field created by the rest of lattice ions over the complex. To illustrate this concept we analyze the origin of the surprisingly large differences in the d–d optical transitions of two systems containing square-planar CuF$_4^{2-}$ complexes, CaCuF$_4$, and center II in Cu$^{2+}$-doped Ba$_2$ZnF$_6$, even though the Cu$^{2+}$–F$^-$ distance difference is just found to be 1%. Using a minimalist first-principles model we show that the different morphology of the host lattices creates an anisotropic field that red-shifts the in vacuo complex transitions to the 1.25–1.70 eV range in CaCuF$_4$, while it blue-shifts them to the 1.70–3.0 eV region in Ba$_2$ZnF$_6$:Cu$^{2+}$. This particular example shows how the lattice anisotropy strongly alters the optical properties of a given transition-metal complex. This knowledge opens a new path to tune the spectra of this large family of systems.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad de Cantabria
Authors: Aramburu, J. A. (Ekstern), García-Fernández, P. (Ekstern), García Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Number of pages: 10
Pages: 8944-8953
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Inorganic Chemistry
Volume: 56
Issue number: 15
ISSN (Print): 0020-1669
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
Lattice constant measurement from electron backscatter diffraction patterns

Kikuchi bands in electron backscattered diffraction patterns (EBSP) contain information about lattice constants of crystallographic samples that can be extracted via the Bragg equation. An advantage of lattice constant measurement from EBSPs over diffraction (XRD) is the ability to perform local analysis. In this study, lattice constants of cubic STN and cubic YSZ in the pure materials and in co-sintered composites were measured from their EBSPs acquired at 10 kV using a silicon single crystal as a calibration reference. The EBSP distortion was corrected by spherical back projection and Kikuchi band analysis was made using in-house software. The error of the lattice constant measurement was determined to be in the range of 0.09–1.12% compared to values determined by XRD and from literature. The confidence level of the method is indicated by the standard deviation of the measurement, which is approximately 0.04 Å. Studying Kikuchi band size dependence of the measurement precision shows that the measurement error decays with increasing band size (i.e. decreasing lattice constant). However, in practice, the sharpness of wide bands tends to be low due to their low intensity, thus limiting the measurement precision. Possible methods to improve measurement precision are suggested.
LCA of Energy Systems

Energy systems are essential in the support of modern societies' activities, and can span a wide spectrum of electricity and heat generation systems and cooling systems. Along with their central role and large diversity, these systems have been demonstrated to cause serious impacts on human health, ecosystems and natural resources. Over the past two decades, energy systems have thus been the focus of more than 1000 LCA studies, with the aim to identify and reduce these impacts. This chapter addresses LCA applications to energy systems for generation of electricity and heat. The chapter gives insight into the LCA practice related to such systems, offering a critical review of (i) central methodological aspects, including the definition of the goals and scopes of the studies, their coverage of the system life cycle and the environmental impacts, and (ii) key findings of the studies, particularly aimed at identifying environmental hotspots and impact patterns across different energy sources. Based on this literature review recommendations and guidelines are issued to LCA practitioners on key methodological aspects that are important for a proper conduct of LCA studies of energy systems and thus ensuring the reliability of the LCA results provided to decision- and policy-makers.

Lead-free, textured piezoelectric ceramics

Main Research Area: Technical/natural sciences

Life cycle assessment of hydrogen production from water electrolysis
Life-Cycle Assessment of Solar Charger with Integrated Organic Photovoltaics

Organic photovoltaics (OPV) applied in a commercial product comprising a solar charged power bank is subjected to a life cycle assessment (LCA) study. Regular power banks harvest electricity from the grid only. The solar power bank (called HeLi-on) is however, a power bank that includes a portable OPV panel, enabling the possibility to be charged from the sun, and not only from the grid. In this paper, two well-established power bank products using amorphous silicon solar panels (a-Si PV) and a regular power bank without any portable solar panel is compared to HeLi-on. The environmental impact of the products is quantified with the aim of indicate where eco-design improvements would make a difference and to point out performance of a portable solar panel depending on the context of use (Denmark and China), realistic disposal scenarios and the recycling relevance particularly concerning metals content.
Lifetime limiting effects in pre-commercial solid oxide cell devices

The solid oxide electrochemical cell technology is promising for efficient energy storage, especially when the share of intermittent renewable electricity production is high. The technology is being commercialized in niche markets, but large-scale employment is still hindered by limited durability of the devices. The lifetime limiting mechanisms are addressed in this work.

A general introduction into mechanisms limiting the durability is presented. A database of more than 50 parameters from 150 publications and 1,000,000 hours of accumulated testing was established, and a quantitative analysis of degradation and lifetime was conducted. It is shown that the technology is approaching the official targets required for commercialization, but that work remains to be done.

It is further recognized that targeting niche applications initially will allow for employment of economies of scale, which will bring down costs and facilitate entry into larger markets. Here, we examine electrochemical reduction of CO2 to CO and one of the main failure mechanisms related to it. Carbon formation on the nickel electrocatalyst can be detrimental to the microstructural integrity of the cell. It is found that the possible operating window is severely limited due to gradients of temperature, gas concentration, and overpotential across the electrode. These affect also apply to stack- and system-level, and the results obtained are combined with modeling and stack testing experiences. Thus, on account of this mechanism the possible outlet CO concentration is limited by up to 50% below the thermodynamic carbon deposition threshold based on the inlet temperature, depending on design and operating strategy.

Replacement of the Ni electrocatalyst would increase the stability towards this issue and may improve the robustness in other ways as well. Ceria has been reported as a potential candidate in such endeavors. Thin film electrodes of nickel and ceria are therefore studied as model systems using near-ambient pressure x-ray photoelectron spectroscopy to further the fundamental understanding of the carbon formation mechanism. The reaction occurs further from the thermodynamic threshold on ceria, and fundamental mechanisms for electrochemically driven carbon growth are suggested based on observed adsorbate species.

By infiltrating ceria after degradation has already occurred, the robustness and lifetime of the cells are increased. Complete reactivation of the fuel electrode isachieved after otherwise detrimental failure mechanisms have occurred, such as reactant starvation and carbon formation. Moreover, the degradation of the electrode over the course of nearly 2500 hours is essentially eliminated by infiltrating after microstructural stabilization had occurred. Lastly, the method is scaled up
by replicating the positive effects of post-degradation infiltration on an 8-cellstack.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Skafte, T. L. (Intern), Hjelm, J. (Intern), Graves, C. R. (Intern)
Number of pages: 142
Publication date: 2017

**Publication information**
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences

**Relations**
Projects:
Lifetime limiting effects in pre-commercial solid oxide cell devices
Publication: Research › Ph.D. thesis – Annual report year: 2017

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**Lithium-Oxygen Batteries: At a Crossroads?**
In this current opinion, we critically review and discuss some of the most important recent findings in the field of rechargeable lithium-oxygen batteries. We discuss recent discoveries like the evolution of reactive singlet oxygen and the use of organic additives to bypass reactive LiO2 reaction intermediates, and their possible implications on the potential for commercialization of lithium-oxygen batteries. Finally, we perform a critical assessment of lithium-superoxide batteries and the reversibility of lithium-hydroxide batteries.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan-Dearborn
Authors: Vegge, T. (Intern), García Lastra, J. M. (Intern), Siegel, D. J. (Intern)
Pages: 100-107
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Current Opinion in Electrochemistry
Volume: 6
ISSN (Print): 2451-9103
Original language: English
DOI: 10.1016/j.coelec.2017.10.014
Publication: Research - peer-review › Journal article – Annual report year: 2017

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**Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole**
Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Søndergaard, T. (Intern), Cleemann, L. N. (Intern), Becker, H. (Intern), Aili, D. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Seerup, L. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: 570-578
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Power Sources
Volume: 342
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Durability, Polymer electrolyte membrane, Fuel cell, Polybenzimidazole, Cross-linking, Thermally cured

DOIs:
10.1016/j.jpowsour.2016.12.075

Source: PublicationPreSubmission
Source-ID: 128050356
Publication: Research - peer-review › Journal article – Annual report year: 2017

Long Term Testing of Solid Oxide Electrolysis Cells under Co-Electrolysis Conditions
Long Term Testing of Solid Oxide Electrolysis Cells Under Co-Electrolysis Conditions

The increasing use of renewables for energy production brings about challenges, for instance, regarding the storage of electricity. Highly efficient solid oxide electrolysis cells (SOECs) can become an attractive solution for converting excess electricity into hydrocarbons (Power-to-Gas). The use of electricity to produce synthetic methane, especially, is considered as a part of the energy transition due to available infrastructure for storage and distribution.

In this contribution, state-of-the-art (SoA) SOECs consisting of a Nickel-Yttria Stabilized Zirconia (Ni-YSZ) fuel electrode, YSZ electrolyte and a mixed ionic electronic conductor (MIEC) Lanthanum Strontium Cobalt Ferrite-Gadolinium doped Ceria (LSCF-GDC) oxygen electrode were tested under co-electrolysis ($H_2O+CO_2$) conditions where the ultimate goal is to produce methane. The SOEC durability tests are traditionally carried out in galvanostatic mode due to the straightforward test control and data interpretation. In this mode, the cell voltages change due to degradation and reach values that are either above or below the thermoneutral voltage which lead to either endothermic or exothermic processes lowering the cell efficiency. However, from a SOEC system point of view, operating the SOEC at thermoneutral voltage (i.e. potentiostatic) is attractive yielding a more efficient system with a comparatively easier heat management. The aim in this study was to compare the SOEC durability under co-electrolysis conditions between galvanostatic and potentiostatic mode. Specifically, the cell was operated at 0.75 A/cm$^2$ (galvanostatic) and at 1.2 V (potentiostatic) at 750 °C for 1000 hours and 500 hours respectively. A detailed electrochemical and microstructure analysis for the two testing regimes will be presented. The degradation mechanisms associated with individual electrode performance will be comprehensively discussed.
Low surface damage dry etched black silicon

Black silicon (bSi) is promising for integration into silicon solar cell fabrication flow due to its excellent light trapping and low reflectance, and a continuously improving passivation. However, intensive ion bombardment during the reactive ion etching used to fabricate bSi induces surface damage that causes significant recombination. Here, we present a process optimization strategy for bSi, where surface damage is reduced and surface passivation is improved while excellent light trapping and low reflectance are maintained. We demonstrate that reduction of the capacitively coupled plasma power, during reactive ion etching at non-cryogenic temperature (-20°C), preserves the reflectivity below 1% and improves the effective minority carrier lifetime due to reduced ion energy. We investigate the effect of the etching process on the surface morphology, light trapping, reflectance, transmittance, and effective lifetime of bSi. Additional surface passivation using atomic layer deposition of Al2O3 significantly improves the effective lifetime. For n-type wafers, the lifetime reaches 12 ms for polished and 7.5 ms for bSi surfaces. For p-type wafers, the lifetime reaches 800 ls for both polished and bSi surfaces.
Low Temperature Synthesis and Properties of Gadolinium-Doped Cerium Oxide Nanoparticles

Gadolinium-doped cerium oxide (GDC) is an attractive ceramic material for solid oxide fuel cells (SOFCs) both as the electrolyte and in composite electrodes operating at low and intermediate temperatures. GDC exhibits high oxygen ion conductivity at a wide range of temperatures and displays a high resistance to carbon deposition when hydrocarbons are used as fuels. However, an inconvenience of ceria-based oxides is the high sintering temperature needed to obtain a fully dense ceramic body. In this study, a green chemistry route for the synthesis of 10 mol% GDC nanoparticles is proposed. The aqueous precipitation method starts from the nitrates of both cerium and gadolinium and uses excess hexamethylenetetramine (HMT) to produce crystalline GDC at 80°C. Such a low temperature synthesis provides control over particle size and sinterability of the material at low temperatures.
Low Temperature Synthesis and Properties of Gadolinium-Doped Cerium Oxide Nanoparticles

Gadolinium-doped cerium oxide (GDC) is an attractive ceramic material for solid oxide fuel cells (SOFCs) both as the electrolyte or in composite electrodes. The Ni/GDC cermet can be tuned as a catalytic layer, added to the conventional Ni/yttria-stabilized zirconia (YSZ), for the internal steam reforming of different fuels. Such an anode allows the SOFC to operate with hydrocarbon fuels by internal reforming. GDC exhibits high oxygen ion conductivity at a wide range of temperatures and displays a high resistance to carbon deposition. However, an inconvenience of ceria-based oxides is the high sintering temperature needed to obtain a fully dense ceramic body, which can result in undesired reactions with YSZ.

In this study, a green chemistry route for the synthesis of 10 mol% GDC nanoparticles is proposed. Such a low temperature synthesis provides control over particle size and sinterability of the material. The aqueous precipitation method starts from the nitrates of both cerium and gadolinium and uses excess hexamethylenetetramine (HMT) to produce crystalline GDC at 80 ºC. As-produced powders were found to be GDC crystalline fluorite-type structure, with crystallite size ≤ 10 nm. Thermalgravimetric analysis show a small mass loss and dilatometry profiles show a total retraction of > 20% up to 1400 ºC. The electrical properties of the material were studied by impedance spectroscopy measurements of sintered samples in a controlled atmosphere. The samples sintered for 2 hours at 1400 ºC exhibited electrical conductivity comparable to previously reported data for GDC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Instituto de Pesquisas Energeticas e Nucleares, Universidade Federal do ABC
Authors: Machado, M. F. S. (Ekstern), P. R. Moraes, L. (Ekstern), Monteiro, N. K. (Ekstern), Esposito, V. (Intern), Zanetti De Florio, D. (Ekstern), Marani, D. (Intern), C. Fonseca, F. (Ekstern)
Pages: 1
Publication date: 2017
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-03
Article number: 322
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/322.abstract
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2017

Luminescence Imaging Strategies for Drone-Based PV Array Inspection

The goal of this work is to develop outdoor defect detection imaging and understand fully its challenges and limitations. The imaging is based on luminescence strategies that will be used for fast and accurate UAV-based inspection system for PV power plants. We studied electroluminescence (EL) acquisition under natural light conditions during several times of the day, under high sun irradiation, to unveil the sunlight noise characteristics towards an InGaAs detector. In order to bring more freedom to a drone-based inspection, we also show the preliminary results of a laser-line based photoluminescence (PL) strategy as a viable method for an outdoor module PL imaging system.

General information
State: Published
Number of pages: 5
Publication date: 2017

Host publication information
Title of host publication: Proceedings of 33rd European Photovoltaic Solar Energy Conference and Exhibition
Main Research Area: Technical/natural sciences
Electroluminescence, Photoluminescence, Defects, Inspections
Magnetic two-dimensional electron gas at the manganite-buffered LaAlO$_3$/SrTiO$_3$ interface

Fabrication of highly mobile spin-polarized two-dimensional electron gas (2DEG) is crucially important for both fundamental and applied research. Usually, spin polarization appears below 10 K for the 2DEG of LaAlO$_3$/SrTiO$_3$ interface, stemming from the magnetic ordering of Ti$^{3+}$ ions with the mediation of itinerant electrons. Herein, we report a magnetic 2DEG at a La$_{7/8}$Sr$_{1/8}$MnO$_3$/SrTiO$_3$ interface, which simultaneously shows electrically tunable anomalous Hall effect and high conductivity. The spin-polarized temperature for the 2DEG is promoted to 30 K while the mobility remains high. The magnetism likely results from a gradient manganese interdiffusion into SrTiO$_3$. The present work demonstrates the great potential of manganite-buffered LaAlO$_3$/SrTiO$_3$ interfaces for spintronic applications.
Mechanical properties of biaxially strained poly(L-lactide) tubes: Strain rate and temperature dependence

Poly(L-lactide) (PLLA) is a bioabsorbable polymer with high stiffness and strength compared to the other commercially available bioabsorbable polymers. The properties of PLLA can be improved by straining, causing deformation-mediated molecular orientation. PLLA tubes were biaxially strained above their $T_g$ for improvement of their strength, in a two-step process (sequential straining). Mechanical properties and crystal morphology were investigated as a function of processing strain rate and temperature. DSC revealed that a low processing strain rate allows molecular chain relaxation in the direction of strain and the crystallization is suppressed. Faster strain rates on the other hand suppress chain relaxation, and results in crystalline tubes. The mechanical properties are influenced by both processing strain rate and temperature. Low strain rates allow chain relaxation resulting in the lowest strength and stiffness, whereas a larger stiffness and strength is achieved by increasing strain rate and temperature. Isotropic mechanical properties are only observed at high processing strain rates.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Amphiphilic Polymers in Biological Sensing, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Wind Energy, Composites and Materials Mechanics, Mixed Conductors
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Polymer Science
Volume: 134
Issue number: 33
Article number: 45192
ISSN (Print): 0021-8995
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.73 SJR 0.532 SNIP 0.724
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.574 SNIP 0.827 CiteScore 1.74
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.658 SNIP 0.964 CiteScore 1.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.628 SNIP 1.085 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.658 SNIP 1.081 CiteScore 1.57
Mechanical Properties of Supports and Half-Cells for Solid Oxide Electrolysis Influenced by Alumina-Zirconia Composites

In order to improve the durability and robustness of solid oxide electrolysis cells (SOEC) and stacks, it is necessary to improve the strength of its components. In cathode supported SOEC, the main structural component is the Ni(O)-YSZ support. But the strength of the half-cell or cell is also determined by the strength of other weaker components and by the residual stress state induced by the thermal expansion mismatch. In this study, the mechanical properties of Ni(O)-3YSZ supports with a reference composition and with substitution of 3YSZ by 20A3YSZ (3YSZ with 20 wt.% Al2O3) have been tested and compared. The initial interest of this substitution are a decrease of the coefficient of thermal expansion (CTE) mismatch within the half-cell and the fact that 20A3YSZ is stronger than 3YSZ. The influence of the process on the composition, strength, elastic properties and electrical conductivity of the supports have been measured and analyzed. The short and long-term evolution of these properties is linked to the formation of a NiAl2O4 phase. The samples were measured at room temperature or high temperature (800 °C) and in oxidized or reduced conditions. The impact of these supports on residual stresses and strength of half-cells is also discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Charlas, B. (Intern), Ni, D. W. (Intern), Frandsen, H. L. (Intern), Brodersen, K. (Intern), Chen, M. (Intern)
Pages: 132-143
Publication date: 2017
Main Research Area: Technical/natural sciences
Metal alloys for the new generation of compressors at hydrogen stations: Parametric study of corrosion behavior

Compressors are one of the most costly components at hydrogen stations, which leads to the high price of hydrogen production. The substitution of a solid piston with an ionic liquid is a promising option that may solve some of the challenges related to conventional reciprocating compressors and, consequently, significantly reduce the final cost of hydrogen production. The correct choice of ionic liquid and construction materials is critical for avoiding significant corrosion problems. Hence, the objective of this study is to evaluate the compatibility of various austenitic stainless steels and nickel-based alloys as construction materials in contact with 80 °C ionic liquids in an ionic liquid hydrogen compressor, considering the role of parameters such as the temperature, viscosity, ionic liquid cation and anion, and water absorption. The results show that temperature contributes to increasing the corrosion rate. However, even at 80 °C, the very low corrosion current densities proved that all of the tested alloys are safe to use as construction materials. AISI 347 showed very high corrosion resistance in all of the ionic liquids. The highest corrosion resistance among all of the tested alloys was observed in trihexyltetradecylphosphonium bis (trifluoromethylsulfonyl) imide, which had a relatively high viscosity and the lowest water content.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Energy Conversion and Storage, Proton conductors
Authors: Arjomand Kermani, N. (Intern), Petrushina, I. (Intern), Nikiforov, A. V. (Intern), Rokni, M. (Intern)
Pages: 805-814
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Renewable Energy
Volume: 116
Issue number: Part A
ISSN (Print): 0960-1481
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.83 SJR 1.697 SNIP 2.044
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.845 SNIP 2.118 CiteScore 4.51
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.687 CiteScore 4.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.066 SNIP 2.767 CiteScore 4.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.852 SNIP 2.745 CiteScore 3.97
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.688 SNIP 2.404 CiteScore 3.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.494 SNIP 2.215
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.305 SNIP 1.945
Web of Science (2009): Indexed yes
Metal–organic frameworks-derived honeycomb-like Co$_3$O$_4$/three-dimensional graphene networks/Ni foam hybrid as a binder-free electrode for supercapacitors

The honeycomb-like porous Co$_3$O$_4$ grown on three dimensional graphene networks/nickel foam (3DGN/NF) has been successfully prepared by a facile solution growth process with subsequent annealing treatment, in which the Co-based metal organic framework (ZIF-67) act as the precursor of the metal oxide. The Co$_3$O$_4$/three-dimensional graphene networks/Ni foam (Co$_3$O$_4$/3DGN/NF) hybrid as the electrode for supercapacitor can deliver high specific capacitance (321 F g$^{-1}$ at 1 A g$^{-1}$) and excellent long-cycling stability (88% of the maximum capacitance after 2000 charge-discharge cycles). Furthermore, the Co$_3$O$_4$/3DGN/NF hybrid exhibits the maximum energy density of 7.5 W h kg$^{-1}$ with the power density of 794 W kg$^{-1}$ and remain 4.1 W h kg$^{-1}$ with the power density of 15 kW kg$^{-1}$ in the two-electrode system. The enhanced electrochemical properties can be attributed to the unique nanostructure of Co$_3$O$_4$ with admirable pseudocapacitance performance and the intimate integration of graphene with the Co$_3$O$_4$ and the Ni foam matrix, which not only enhances the electron conductivity for fast electron and ion transport but also provides high specific surface area and excellent structural stability.
Micromechanics Models for Viscoelastic Plain-Weave Composite Tape Springs

The viscoelastic behavior of polymer composites decreases the deployment force and the postdeployment shape accuracy of composite deployable space structures. This paper presents a viscoelastic model for single-ply cylindrical shells (tape springs) that are deployed after being held folded for a given period of time. The model is derived from a representative unit cell of the composite material, based on the microstructure geometry. Key ingredients are the fiber volume density in the composite tows and the constitutive behavior of the fibers (assumed to be linear elastic and
transversely isotropic) and of the matrix (assumed to be linear viscoelastic). Finite-element-based homogenizations at two scales are conducted to obtain the Prony series that characterize the orthotropic behavior of the composite tow, using the measured relaxation modulus of the matrix as an input. A further homogenization leads to the lamina relaxation ABD matrix. The accuracy of the proposed model is verified against the experimentally measured time-dependent compliance of single lamina in either pure tension or pure bending. Finite element simulations of single-ply tape springs based on the proposed model are compared to experimental measurements that were also obtained during this study.
Microscopic origin of the mobility enhancement at a spinel/perovskite oxide heterointerface revealed by photoemission spectroscopy

The spinel/perovskite heterointerface γ-Al₂O₃/SrTiO₃ hosts a two-dimensional electron system (2DES) with electron mobilities exceeding those in its all-perovskite counterpart LaAlO₃/SrTiO₃ by more than an order of magnitude, despite the abundance of oxygen vacancies which act as electron donors as well as scattering sites. By means of resonant soft x-ray photoemission spectroscopy and ab initio calculations, we reveal the presence of a sharply localized type of oxygen vacancies at the very interface due to the local breaking of the perovskite symmetry. We explain the extraordinarily high mobilities by reduced scattering resulting from the preferential formation of interfacial oxygen vacancies and spatial separation of the resulting 2DES in deeper SrTiO₃ layers. Our findings comply with transport studies and pave the way towards defect engineering at interfaces of oxides with different crystal structures.
Microstructural and electrical characterization of Mn-Co spinel protective coatings for solid oxide cell interconnects

Electrophoretic deposition, thermal co-evaporation and RF magnetron sputtering methods are used for the preparation of Mn-Co based ceramic coatings for solid oxide fuel cell steel interconnects. Both thin and relatively thick coatings (1–15 μm) are prepared and characterised for their potential protective behaviour. Mn-Co coated Crofer22APU samples are electrically tested for 5000 h at 800 °C under a 500 mA cm⁻² current load to determine their Area Specific Resistance increase due to a growing chromia scale. After tests, samples are analysed by scanning and transmission electron microscopy. Analysis is focused on the potential chromium diffusion to or through the coating, the oxide scale thickness and possible reactions at the interfaces. The relationships between the coating type, thickness and effectiveness are reviewed and discussed. Out of the three Mn-Co coatings compared in this study, the one deposited by electrophoretic deposition presents the best protection against Cr diffusion and offers long term stability.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Politecnico di Torino, Edison Research & Development Center, AGH University of Science and Technology, University of Erlangen-Nuremberg
Authors: Molin, S. (Intern), Sabato, A. G. (Ekstern), Bindi, M. (Ekstern), Leone, P. (Ekstern), Cempura, G. (Ekstern), Salvo, M. (Ekstern), Cabanas Polo, S. (Ekstern), Boccaccini, A. R. (Ekstern), Smeacetto, F. (Ekstern)
Pages: 4781-4791
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 15
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.392 SNIP 1.945
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.381 SNIP 1.724
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BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.146 SNIP 1.645
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.22 SNIP 1.76
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.191 SNIP 1.67
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.084 SNIP 1.637
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.037 SNIP 1.747
Scopus rating (2003): SJR 1.129 SNIP 1.497
Scopus rating (2002): SJR 1.04 SNIP 1.181
Scopus rating (2001): SJR 1.238 SNIP 1.597
Scopus rating (2000): SJR 0.99 SNIP 1.182
Scopus rating (1999): SJR 1.141 SNIP 1.156
Original language: English
Solid oxide cell, Electrophoretic deposition, Protective coating, Area specific resistance, Microstructure
DOIs:
Microstructural Characterization of Ni/YSZ Electrodes in a Solid Oxide Electrolysis Stack Tested for 9000 Hours
The effects of long-term operation in electrolysis mode on the microstructure of Ni/YSZ electrodes were investigated. The electrode structures were investigated in "as reduced" state and after 9000 h of operation in a 25 cell stack. Microstructural data were obtained by scanning electron microscopy and focused-ion-beam serial sectioning. Microstructural characteristics were extracted by 1D and 3D methods. Significant microstructural changes were observed between the two cells analyzed. A significant loss of Ni in the active electrode is observed, from ~ 29% (by volume) in the reference cell to ~ 24% as well as a coarsening of the Ni particle sizes. The long-term tested cell shows lower percolating triple phase boundary density (0.76 µm/µm³) than the un-tested reference (2.0 µm/µm³). This reduction is mainly due to the loss of triple phase boundary percolation through the Ni phase where a reduction from a percolation degree above 90% to ~50% is observed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Trini, M. (Intern), Jørgensen, P. S. (Intern), Hauch, A. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Pages: 3049-3064
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
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Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
Electronic versions:
ECSTransaction_martina_trini_post_print_from_DTU_Energy.pdf
DOIs:
Microstructural Characterization of Ni/YSZ Electrodes in a Solid Oxide Electrolysis Stack Tested for 9000 Hours

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Trini, M. (Intern), Jørgensen, P. S. (Intern), Hauch, A. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: Electrochemical Society, Incorporated
Article number: 201
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/201

Microstructure and chemical data of the thermoelectric ZnSb material after joining to metallic electrodes and heat treatment
The data presented in this article are related to the research article entitled: “Solder free joining as a highly effective method for making contact between thermoelectric materials and metallic electrodes” (Malik et al., 2017) [1]. This article presents microstructure obtained by scanning electron microscopy (SEM) and chemical analysis by energy dispersive X-ray spectroscopy (EDX) point measurements of the thermoelectric ZnSb legs after joining to metallic electrodes using solder (Zn-2Al) and free-soldering methods.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Authors: Malik, S. A. (Intern), Le, T. H. (Intern), Van Nong, N. (Intern)
Pages: 97-101
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Data in Brief
Volume: 15
ISSN (Print): 2352-3409
Ratings:
Scopus rating (2016): CiteScore 0.5 SJR 0.216 SNIP 0.201
Scopus rating (2015): SJR 0.186 SNIP 0.065 CiteScore 0.25
Original language: English
Electronic versions:
1_s2.0_S2352340917304547_main.pdf
1_s2.0_S2352340917304547_main.pdf
DOIs:
10.1016/j.dib.2017.09.023
Source: PublicationPreSubmission
Source-ID: 137100446
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Microstructure and Electrical Properties of Fe,Cu Substituted (Co,Mn)₃O₄ Thin Films
In this work, thin films (~1000 nm) of a pure MnCo₂O₄ spinel together with its partially substituted derivatives (MnCo₁.₆₋ₓCuₓFeₓO₄, MnCo₁.₆₋ₓCuₓO₄, MnCo₁.₆₋ₓFeₓO₄) were prepared by spray pyrolysis and were evaluated for electrical conductivity. Doping by Cu increases the electrical conductivity, whereas doping by Fe decreases the conductivity. For Cu
containing samples, rapid grain growth occurs and these samples develop cracks due to a potentially too high thermal expansion coefficient mismatch to the support. Samples doped with both Cu and Fe show high electrical conductivity, normal grain growth and no cracks. By co-doping the Mn, Co spinel with both Cu and Fe, its properties can be tailored to reach a desired thermal expansion coefficient/electrical conductivity value.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Szymczewska, D. (Ekstern), Molin, S. (Intern), Hendriksen, P. V. (Intern), Jasinski, P. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

**Mid-IR optical properties of silicon doped InP**

InP is one of the most important materials for optoelectronics as a direct bandgap semiconductor, which can also be regarded as a low loss alternative plasmonic material for mid-infrared (mid-IR). The InP films studied in this work were grown by metal-organic vapor phase epitaxy (MOVPE). The effect of growth conditions on the optical and electrical properties of silicon doped InP (InP:Si) in the wavelength range from 3 to 40 μm was studied. The carrier concentration of up to $3.9 \times 10^{19} \text{ cm}^{-3}$ is achieved by optimizing the growth conditions. The dielectric function, effective mass of electrons and plasma frequency were determined by Fourier transform infrared spectroscopy (FTIR) for different carrier density levels. The plasma frequency can be tuned effectively via doping from 18.43 to 50.5 THz. Based on the experimental results, a semi-empirical formula for the plasma frequency, as a function of carrier concentration, is derived. Comparison to other semiconductors shows superior plasmonic performance of InP:Si in terms of propagation length and surface confinement.

**General information**

State: Published
Organisations: Plasmonics and Metamaterials, Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Department of Photonics Engineering, Nanophotonic Devices, Centre of Excellence for Silicon Photonics for Optical Communications, St. Petersburg Academic University
Authors: Panah, M. E. A. (Intern), Han, L. (Intern), Norman, K. (Intern), Pryds, N. (Intern), Nadtochiy, A. (Ekstern), Zhukov, A. E. (Ekstern), Lavrinenko, A. (Intern), Semenova, E. (Intern)
Pages: 2260-2271
Publication date: 2017
Main Research Area: Technical/natural sciences
Model for solid oxide fuel cell cathodes prepared by infiltration

A 1-dimensional model of a cathode has been developed in order to understand and predict the performance of cathodes prepared by infiltration of La0.6Sr0.4Co1.05O3-δ (LSC) into porous backbones of Ce0.9Gd0.1O1.95 (CGO). The model accounts for the mixed ionic and electronic conductivity of LSC, ionic conductivity of CGO, gas transport in the porous cathode, and the oxygen reduction reaction at the surface of percolated LSC. Geometrical variations are applied to reflect a changing microstructure of LSC under varying firing temperatures. Using microstructural parameters obtained from detailed scanning electron microscopy and simulations of the measured polarization resistances, an expression for the area specific resistance (rp) associated with the oxygen exchange on the surface of the infiltrated LSC particles was extracted and compared with literature values. A series of microstructural parameter variations are presented and discussed with the aim of presenting specific guidelines for optimizing the microstructure of cathodes prepared by infiltration.
Modeling a material from packing, through sintering and to the final microstructural properties

We present a combination of numerical models that can together simulate the initial packing of particles, followed by sintering and finally the resulting microstructural properties. For the latter we here focus on the magnetism of a sintered sample, and the associated coupling between heat and magnetism known as the magnetocaloric effect. We present a 3-dimensional time-dependent numerical model that spatially resolves samples down to the grain size, and includes the demagnetizing field, chemical inhomogeneity realized as a spatial variation of Curie temperature across the sample, local hysteresis and heat transfer. We can thus model how particle size, packing, sintering and chemical inhomogeneity affect the observed properties of magnetocaloric samples. For example, we show that even a modest distribution in Curie temperature (TC) across the sample results in a significant broadening and lowering of the total entropy change of the sample around TC. We discuss how clustering of grains with similar values of TC across the sample influences the results.
Modeling of Ni Diffusion Induced Austenite Formation in Ferritic Stainless Steel Interconnects

Ferritic stainless steel interconnect plates are widely used in planar solid oxide fuel cell and electrolysis cell stacks. During stack production and operation, nickel from the Ni/yttria stabilized zirconia fuel electrode or from the Ni contact component layer diffuses into the interconnect plate, causing transformation of the ferritic phase into an austenitic phase in the interface region. This is accompanied with changes in volume, and in mechanical and corrosion properties of the interconnect plates. In this work, kinetic modeling of the inter-diffusion between Ni and FeCr based ferritic stainless steel was conducted, using the CALPHAD (CALculation of PHAse Diagrams) approach with the DICTRA (Diffusion Controlled TRAnsformation) software. The kinetics of inter-diffusion and austenite formation was explored in detail. The simulation was further validated by comparing with experiments. The results show that after 2000 h at 800°C Ni diffuses more than 100 μm deep into Crofer 22 APU. Along with the Ni diffusion, part of the ferritic steel with 50–60 μm in thickness has transformed into the austenitic phase. Growth of the austenite phase in commercial interconnect materials was predicted to take place under practical stack operation conditions.
We developed an improved model to fit the photocurrent density versus voltage in organic solar cells. The model has been validated by fitting data from P3HT:PCBM solar cells. Our model quantitatively accounts for the band bending near the electrodes caused by charge accumulation in the active layer. The model explains the position of the built-in and the zero-field voltage, the value of the internal electric field, the impact of electrode materials, and the appearance of multiple inflections. In addition, the model can be used to monitor the cell condition during accelerated lifetests.

Model of Organic Solar Cell Photocurrent Including the Effect of Charge Accumulation at Interfaces and Non-Uniform Carrier Generation

We developed an improved model to fit the photocurrent density versus voltage in organic solar cells. The model has been validated by fitting data from P3HT:PCBM solar cells. Our model quantitatively accounts for the band bending near the electrodes caused by charge accumulation in the active layer. The model explains the position of the built-in and the zero-field voltage, the value of the internal electric field, the impact of electrode materials, and the appearance of multiple inflections. In addition, the model can be used to monitor the cell condition during accelerated lifetests.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padua
Authors: Torto, L. (Ekstern), Cester, A. (Ekstern), Rizzo, A. (Ekstern), Wrachien, N. (Ekstern), Gevorgyan, S. (Intern), Corazza, M. (Intern), Krebs, F. C. (Intern)
Pages: 387-395
Publication date: 2017
Main Research Area: Technical/natural sciences
Molecular dynamics simulation of radiation grafted FEP films as proton exchange membranes: Effects of the side chain length

In order to study the microstructure of the prepared potential proton exchange membrane (PEM), molecular dynamics (MD) simulations were used to elucidate the transport behavior of water molecules and hydronium ions inside the hydrated sulfonated styrene grafted fluorinated ethylene propylene (FEP) membrane, which possess different side chain lengths. By evaluating the radial distribution functions (RDFs), it was observed that with increasing side chain length, the average sulfur-hydronium ion separation slightly increased and the coordination number of H3O+ around sulfonic acid groups decreased whereas larger water clusters formed. The results of the mean square displacements (MSDs) show that the proton conductivities of the membranes with the proposed side chain lengths were about three fifths of the experimental data, of which the membrane with side chain length of 7 sulfonic styrene units was supposed to exhibit the highest proton conductivity, that is 115.69 mS cm⁻¹. All of the supposed membrane models presented good proton conductivity that could definitely meet the application requirements of the proton exchange membranes. The MD simulations can provide an insight to the chain structure of the radiation grafted membrane, and are of guidance significance to design other side-chain-structure polymers to be used as PEMs in proton exchange membrane fuel cells (PEMFCs).
Mononuclear Clusterfullerene Single-Molecule Magnet Containing Strained Fused-Pentagons Stabilized by a Nearly Linear Metal Cyanide Cluster

Fused-pentagons result in an increase of local steric strain according to the isolated pentagon rule (IPR), and for all reported non-IPR clusterfullerenes multiple (two or three) metals are required to stabilize the strained fused-pentagons, making it difficult to access the single-atom properties. Herein, we report the syntheses and isolations of novel non-IPR mononuclear clusterfullerenes MNC@C76 (M=Tb, Y), in which one pair of strained fused-pentagon is stabilized by a mononuclear cluster. The molecular structures of MNC@C76 (M=Tb, Y) were determined unambiguously by single-crystal X-ray diffraction, featuring a non-IPR C2v(19138)-C76 cage entrapping a nearly linear MNC cluster, which is remarkably different from the triangular MNC cluster within the reported analogous clusterfullerenes based on IPR-obeying C82 cages. The TbNC@C76 molecule is found to be a field-induced single-molecule magnet (SMM).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Science and Technology of China, Xiamen University, University of Science and Technology of China, Universität Zürich, Leibniz Institute for Solid State and Materials Research Dresden
Authors: Liu, F. (Ekstern), Wang, S. (Ekstern), Gao, C. L. (Ekstern), Deng, Q. (Intern), Zhu, X. (Ekstern), Kostanyan, A. (Ekstern), Westerstroem, R. (Ekstern), Jin, F. (Ekstern), Xie, S. Y. (Ekstern), Popov, A. A. (Ekstern), Greber, T. (Ekstern), Yang, S. (Ekstern)
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<td>2004</td>
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Near-net shape manufacture of B4C–Co and ZrC–Co composites by slip casting and pressureless sintering

Fabrication of near-net shaped B4C–Co and ZrC–Co composites by slip casting and pressureless sintering is described. It is shown how B4C–Co and ZrC–Co concentrated suspensions can be prepared by aqueous colloidal processing, and optimized (in terms of pH, deflocculant contents, and sonication time) to have a shear-thinning rheological behaviour suitable for the near-net shaping of the corresponding cermet compacts by slip casting. It is also demonstrated that the robust, highly-dense compacts so obtained have a uniform green microstructure without macro-defects or gradient density, and which can be fully densified by pressureless sintering. Specifically, it is shown that B4C–Co compacts densify by reactive and transient liquid-phase sintering, thus resulting in multi-component ceramics. ZrC–Co compacts densify however by persistent liquid-phase sintering, thus resulting in cermets. An explanation is given for these observations, and general implications are discussed for the near-net shape manufacture of these and similar carbide-metal composites for use in engineering applications.
New Light Source Setup for Angle Resolved Light Absorption measurement of PV sample

Here, we introduce measurements of angle resolved light absorption by PV cells, using broadband laser driven white light source with a bright, stable, broad spectral range and well collimated light.
NOx Selective Catalytic Reduction (SCR) on Self-Supported V-W-doped TiO2 Nanofibers

Electrospun V–W–TiO2 catalysts, resulting in a solid solution of V and W in the anatase phase, are prepared as nonwoven nanofibers for NOx selective catalytic reduction (SCR). Preliminary catalytic characterization indicates their superior NOx conversion efficiency to the state-of-the-art material. A novel concept of a self-supported, ultra-compact, and lightweight nanofibrous SCR-reactor is defined.
Nucleophilic stabilization of water-based reactive ink for titania-based thin film inkjet printing

Drop on demand deposition (DoD) of titanium oxide thin films (<500 nm) is performed via a novel titanium-alkoxide-based solution that is tailored as a reactive ink for inkjet printing. The ink is developed as water-based solution by a combined use of titanium isopropoxide and n-methyldiethanolamine (MDEA) used as nucleophilic ligand. The function of the ligand is to control the fast hydrolysis/condensation reactions in water for the metal alkoxide before deposition, leading to formation of the TiO₂ only after the jet process. The evolution of the titanium-ligand interactions at increasing amount of MDEA is here elucidated in terms of long term stability. The ink printability parameter (Z) is optimized, resulting in a reactive solution with printability, Z, >1, and chemical stability up to 600 h. Thin titanium oxide films (<500 nm) are proved on different substrates. Pure anatase phase is obtained after annealing at low temperature (ca. 400 °C).
Numerical routine for magnetic heat pump cascading

Heat pumps use low-temperature heat absorbed from the energy source to create temperature gradient (TG) across the energy sink. Magnetic heat pumps (MHP) can perform this function through operating active magnetic regeneration (AMR) cycle. For building heating, TGS of up to a few K might be necessary, which is hardly achievable with a single MHP and such techniques as cascading are required. Series and parallel cascading increase the AMR span and heating power, respectively, but do not change TG. Therefore, the intermediate type of cascading was proposed with individual MHPs separately connected at their cold and hot sides [1]. In these works, a single MHP is separated into smaller cascaded MHPs with the same total mass. This kind of mass redistribution is hard to implement experimentally since several prototypes with different AMR number and sizes should be constructed. In this theoretical study, instead of changing individual AMR sizes, we rearranged parallel-connected AMRs in separate blocks (HP1, HP2 and HP3 in Fig. 1(a)) and connected the cold (hot) outlet of one block to the cold (hot) inlet of the next block giving a cascading configuration. Thus, not only the total mass but also the total number of AMRs remain constant, making this configuration easier to implement. A MATLAB routine for cascading simulation from a single AMR data was implemented. Calculated heating power for configuration in Fig. 1(a) is plotted in Fig. 1(b) and the cold- and hot-side TGS are around 2 K and 3 K. Changing the number of MHPs, we optimized input parameters to achieve maximum heating powers. We have found that both maximum heating power and COP decrease together with number of heat pumps, but the TGS and the temperature span can be largely increased. References [1] M. Tahavori et al., “A Cascading Model Of An Active Magnetic Regenerator System”, In Proceedings of the 7th International Conference on Magnetic Refrigeration at Room Temperature (2016) 248-251

General information
Numerical simulation of kinetic demixing and decomposition in a LaCoO$_{3-\delta}$ oxygen membrane under an oxygen potential gradient

A composition- and temperature-dependent mobility database of all ionic species in the LaCoO$_{3-\delta}$ phase was developed and combined with a La-Co-O thermodynamic database to simulate kinetic demixing and partial decomposition in LaCoO$_{3-\delta}$ oxygen membranes operated under a 0.0001/0.21 bar oxygen partial pressure difference at 1073 K for 1 year. Formation of La$_2$O$_3$, Co$_3$O$_4$, and CoO phases across the membrane is predicted. The kinetic demixing process can be divided into two steps, namely, establishment of the oxygen potential gradient (fast) and demixing of the cations (slow); the former is controlled by the mobility of oxygen ions, and the latter is determined by the higher mobility of Co ions as compared to the La ion in the ABO$_3$-type perovskite. A drift motion of both oxide surfaces towards the high $P_{O_2}$ side occurs with the movement of cations.

General information

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Central South University
Number of pages: 24
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Membrane Science
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2 SNIP 1.771 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.433 SNIP 1.935 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.452 SNIP 2.001 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.201 SNIP 1.968 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.82 SNIP 1.726 CiteScore 4.29
On the Properties and Long-Term Stability of Infiltrated Lanthanum Cobalt Nickelates (LCN) in Solid Oxide Fuel Cell Cathodes

Infiltration as a fabrication method for solid oxide fuel cells (SOFC) electrodes is offering significant improvements in cell performance at reduced materials and fabrication costs, especially when combined with co-sintering. However, important questions regarding the long-term performance and microstructural stability remain unanswered. Here, we present the results of a three-year project, where large footprint anode-supported SOFCs with a co-sintered cathode backbone and infiltrated La0.95Co0.4Ni0.6O3 (LCN) cathodes were developed and thoroughly characterized. The initial long-term performance and stability of this new cell type was investigated for 1500+ hours, coupled with STEM-EDS investigation of the microstructural changes in the infiltrated electrodes. Additionally, electrodes were further aged at elevated temperatures (750 - 900°C) for periods reaching up to 5000 hours, while following changes in the electrode properties using SEM, BET area, and in-plane conductivity measurements. Finally, the mechanical properties of co-sintered cathode backbone cells were determined in four-point bending tests carried out both at room temperature and at 800°C in air. Based on these results, degradation mechanisms were identified and recommendation for safe operation conditions in real life application could be formulated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Fundamental Electrochemistry, Imaging and Structural Analysis, Haldor Topsoe AS
Pages: F748-F758
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 164
On the way towards smart energy supply in cities: The impact of interconnecting geographically distributed district heating grids on the energy system

A linear continuous optimization model with an hourly time resolution was developed in order to model the impact of subsequent interconnections of different DH grids. The municipality of Sønderborg was chosen for a case study and interconnections of five currently disconnected DH grids were assessed. Moreover, the impact of industrial waste heat on the DH supply was also assessed. In the reference year (2013) two out of four interconnections proved to be economically viable. The results for the future energy system (2029) showed that interconnecting geographically distributed DH grids reduces primary energy supply by 9.5%, CO₂ emissions by 11.1% and total system costs by 6.3%. Inclusion of industrial waste heat in the fully interconnected DH grid reduced primary energy supply for an additional 3%, CO₂ emissions for an additional 2.2% and total system costs for an additional 1.3%. The case of the future energy supply system with interconnected DH grids and installed industrial waste heat recuperation results in the lowest primary energy demand, emissions and costs. Finally, the benefits of the interconnected DH grid, in terms of system flexibility, CO₂ emissions, total costs and energy efficiency, proved to be much greater in the future energy system.
Operational test of bonded magnetocaloric plates

Bonded plates made by hot pressing La$_{0.85}$Ce$_{0.15}$Fe$_{11.25}$Mn$_{0.25}$Si$_{1.5}$H$_x$ particles and resin have been tested as active magnetic regenerators in a small scale magnetocaloric device. Firstly the plates were carefully characterised magnetically and thermally. The plates were prepared with 5 wt% resin, and from density measurements it was found that the volume ratio of the magnetocaloric material in the plates was 0.53, due to the resin and porosity. The best operating conditions for the plate regenerator were determined at which a temperature span of 6.4 K was measured along the plates.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences, University of Science and Technology Beijing
Pages: 245-251
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Refrigeration
Volume: 76
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Orientation-Dependent Oxygen Evolution on RuO₂ without Lattice Exchange

RuO₂ catalysts exhibit record activities toward the oxygen evolution reaction (OER), which is crucial to enable efficient and sustainable energy storage. Here we examine the RuO₂ OER kinetics on rutile (110), (100), (101), and (111) orientations, finding (100) the most active. We assess the potential involvement of lattice oxygen in the OER mechanism with online electrochemical mass spectrometry, which showed no evidence of oxygen exchange on these oriented facets in acidic or basic electrolytes. Similar results were obtained for polyoriented RuO₂ films and particles, in contrast to previous work, suggesting lattice oxygen is not exchanged in catalyzing OER on crystalline RuO₂ surfaces. This hypothesis is supported by the correlation of activity with the number of active Ru-sites calculated by density functional theory, where more active facets bind oxygen more weakly. This new understanding of the active sites provides a design strategy to enhance the OER activity of RuO₂ nanoparticles by facet engineering.
**Overcoming the Scaling Lag for Polymer Solar Cells**

There is a long stretch between a laboratory discovery and a practical demonstration. For a potentially useful energy technology, many further strides must be taken before a societally meaningful scale is reached. In this work we have, based on many past experiences, brought the fully roll-to-roll printed polymer solar cell to a realistic scale across the entire value chain. The materials synthesis, the manufacture, the installation, the failure modes, and the operation have all been covered and addressed. We demonstrate outdoor operation for 2 years through a large-scale, grid-tied, high-voltage system and show that thin plastic foil can be operated as an energy-producing technology. Critical to the demonstration was the identification of the drying method during printing, and we show how this development relates to the scaling lag (the period between the point in time for a laboratory demonstration and the point in time for scaled manufacture) and allows for closure of the scaling gap.

**Oxide Modules**

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science


Pages: 274-289
Publication date: 2017
Main Research Area: Technical/natural sciences
The perovskite-type oxide (La0.6Ca0.4)(Co0.8Fe0.2)O3-δ (LCCF) was investigated for use as oxygen separation membrane. A 25 µm thick dense membrane on a porous LCCF support with a thickness of around 175 µm was prepared by a tape casting and lamination process. The optimum sintering temperature of the component was established to be 1050 °C by analysis of microstructures of membranes sintered at different temperatures. Scanning electron microscopy (SEM) examination of cross-sections of the sintered membrane showed that it consisted of two phases, the main phase being enriched in calcium (Ca) and depleted in lanthanum (La), relative to the nominal composition. A surface activation layer of LCCF was deposited onto the dense layer to increase the exchange rate of oxygen at the surface. For the coated membrane, the oxygen permeation flux increased with temperature and reached a maximum value of 3.32 Nml cm⁻² min⁻¹ at 900 °C when, for characterization purpose pure oxygen was used as feed and a maximum value of 2.06 Nml cm⁻² min⁻¹ at 900 °C was obtained when air was used at the feed side, both with N₂ sweep on the permeate side. The stability of the membrane against sulfur dioxide (SO₂) and pure carbon dioxide (CO₂) was tested. A small decrease in the flux was observed over 48 h in CO₂ at 850 °C. SEM examinations of the cross-section of the tested membrane showed that the Ca rich phase in the membrane showed a tendency to migrate to the feed side. Whereas the material shows a CO₂ stability superior to that of Sr or Ba containing analogues, the material stability is not sufficient for applications requiring direct exposure to sulfur-rich flue gases.
Oxygen permeation membrane, Kinetic demixing, Stability, Oxy-fuel

DOIs:
10.1016/j.memsci.2017.07.050

Source: PublicationPreSubmission
Source-ID: 134380925
Publication: Research - peer-review › Journal article – Annual report year: 2017

Oxygen permeation membrane, Kinetic demixing, Stability, Oxy-fuel

Oxygen transport properties of tubular $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95}\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_{3-d}$ composite asymmetric oxygen permeation membranes supported on magnesium oxide

The oxygen permeation through dense $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95}\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_{3-d}$ dual-phase composite asymmetric membranes supported on a porous MgO tube was studied. The membranes were prepared by thermoplastic extrusion, dip coating, co-sintering and infiltration of a catalyst. Oxygen permeation measurements and electrical conductivity characterization of the membrane were performed as a function of temperature and oxygen partial pressure. The oxygen flux through the membrane in a H$_2$/air gradient at 850 °C reached 15 N ml cm$^{-2}$ min$^{-1}$. The measured oxygen flux was in good agreement with the theoretically estimated one, taking into account the transport properties of the composite, surface exchange losses, gas diffusion and gas conversion in the MgO support. The performance of the membrane was limited by the surface exchange for the operation in N$_2$/air, CO$_2$/air and H$_2}$/air at low temperatures and most probably by the porosity of the MgO support for the operation in H$_2}$/air at 850 °C. The stability tests of the membrane in CO$_2}$/air and H$_2}$/air configurations revealed that an initial degradation of the oxygen flux occurs and it is followed by a relatively stable performance. Post-mortem analysis of the membrane after 900 h of operation did not reveal any significant microstructural degradation of the membrane layer.

General information
State: Published
PALSfit3: A software package for analysing positron lifetime spectra

The present report describes a Windows based computer program called PALSfit3. The purpose of the program is to carry out analyses of spectra that have been measured by positron annihilation lifetime spectroscopy (PALS). PALSfit3 is based on the well tested PATFIT and PALS fit programs, which have been used extensively by the positron annihilation community. The present document describes the mathematical foundation of the PALSfit3 model as well as a number of features of the program. The cornerstones of PALSfit3 are two least squares fitting modules: POSITRONFIT and RESOLUTIONFIT. In both modules a model function will be fitted to a measured lifetime spectrum. This model function consists of a function representing the physics of the positron decay which is convoluted with the experimental time resolution function, plus a constant background. The 'physics function' consists of a sum of decaying exponentials each of which may be broadened by convolution with a log-normal lifetime distribution. The time resolution function is described by a sum of Gaussians which may be displaced with respect to each other. Various types of constraints may be imposed on the fitting parameters. In the POSITRONFIT module, the fitting parameters to be extracted from a measured spectrum are for each lifetime component its mean lifetime and its broadening as well as its intensity. A correction for positrons annihilating outside the sample can be made as part of the analysis. In the RESOLUTIONFIT module, parameters determining the shape of the time resolution function can be fitted. The extracted resolution function may then be used in POSITRONFIT.

Graphics displays are provided to ease the selection of some of the input parameters and to display results of spectrum analysis. The results are also available in a text window. PALSfit3 is verified on Windows XP and Windows 7, 8 and 10. The PALSfit3 software can be acquired from the Technical University of Denmark (http://PALSfit.dk)

General information
State: Published
Organisations: Department of Energy Conversion and Storage, IT Service
Authors: Kirkegaard, P. (Intern), Olsen, J. V. (Intern), Eldrup, M. M. (Intern)
Number of pages: 59
Publication date: 2017

Publication information
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
ISBN (Print): 978-87-92986-61-0
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: palsfit3_final.pdf
Source: PublicationPreSubmission
Source-ID: 130449192
Publication: Research › Report – Annual report year: 2017

Passive characterization and active testing of epoxy bonded regenerators for room temperature magnetic refrigeration

Epoxy bonded regenerators of both spherical and irregular La(Fe,Mn,Si)_{13}H_y particles have been developed aiming at increasing the mechanical strength of active magnetic regenerators (AMR) loaded with brittle magnetocaloric materials and improving the flexibility of shaping the regenerator geometry. Although the magnetocaloric properties of these materials are well studied, the flow and heat transfer characteristics of the epoxy bonded regenerators have seldom been investigated. This paper presents a test apparatus that passively characterizes regenerators using a liquid heat transfer fluid with an oscillating flow at low Reynolds numbers, simulating the hydraulic working conditions in AMRs. Dimensionless parameters, including friction factor, effectiveness and overall Nusselt number, are presented for the epoxy bonded La(Fe,Mn,Si)_{13}H_y regenerators and reference packed particle beds. Moreover, a five-layer AMR based on spherical particles is tested actively in a small reciprocating magnetic refrigerator, achieving a no-load temperature span of 16.8 °C.
using about 143 g of epoxy-bonded La(Fe,Mn,Si)$_{13}$H$_y$ materials. Simulations based on a one-dimensional (1D) AMR model are also implemented to validate and analyze the results from the active test.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Vacuumschmelze GmbH & Co. KG
Authors: Lei, T. (Intern), Navickaitė, K. (Intern), Engelbrecht, K. (Intern), Barcza, A. (Ekstern), Vieyra, H. (Ekstern), Nielsen, K. K. (Intern), Bahl, C. (Intern)
Pages: 10-19
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Applied Thermal Engineering
Volume: 128
ISSN (Print): 1359-4311
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.78 SJR 1.462 SNIP 1.828
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.734 SNIP 1.898 CiteScore 3.32
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.576 SNIP 2.206 CiteScore 3.16
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.516 SNIP 2.5 CiteScore 3.31
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.54 SNIP 2.432 CiteScore 2.7
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.389 SNIP 2.186 CiteScore 2.83
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.425 SNIP 2.045
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.435 SNIP 2.126
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.194 SNIP 1.66
- Scopus rating (2007): SJR 0.892 SNIP 1.479
- Scopus rating (2006): SJR 1.221 SNIP 1.582
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.17 SNIP 1.445
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.986 SNIP 1.273
- Scopus rating (2003): SJR 0.916 SNIP 1.134
- Scopus rating (2002): SJR 0.878 SNIP 1.005
Pd Nanoparticles-Supported Carbon Nanotube-Encapsulated NiO/MgO Composite as an Enhanced Electrocatalyst for Ethanol Electrooxidation in Alkaline Medium

In this work, an easy method is developed to prepare well-dispersed palladium nanoparticles into the carbon nanotube (CNT) encapsulated NiO/MgO nanocomposite by the chemical reduction method. CNT encapsulated NiO/MgO nanocomposite were prepared by autogenous pressure at elevated temperature (RAPET) method. The Pd/(NiO/MgO-CNT) catalyst was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), higher resolution-transmission electron microscopy (HR-TEM), Raman spectroscopy and electrochemical analysis. Electrochemical measurements demonstrate the as synthesized Pd/(NiO/MgO-CNT) catalysts exhibit superior electrochemical performance compare to the commercial Pd/C catalysts. The current densities of the main anodic peak of electrooxidation of ethanol increases sharply for the Pd/(NiO/MgO-CNT) (98.20 mA/cm²), which are ~2.1 times as large as that of Pd/C (47 mA/cm²). The excellent electrochemical performance can be attributed on the one hand to the incorporation of NiO/MgO on palladium on the other hand to the porous tubular morphology of the CNT leads to high dispersion of Pd nanoparticles and also enhances the mass transport of the electrode.

Performance and electrochemical analysis of solid oxide fuel cells based on LSCF-YSZ nano-electrode

NiO-YSZ/YSZ/LSCF-YSZ tri-layer structure SOFC has been fabricated by tape casting and infiltration methods. Subsequently, polarization curves and electrochemical impedance spectra measurement were carried out to evaluate cell performance at 850-700°C with varied steam content in hydrogen supplied to the anode. At 800°C, open circuit voltage for 4% steam-humidified hydrogen reached 1.069 V, along with a power density of 831 mW/cm² at 0.7 V. Furthermore, 500 hours of long-term durability test has been performed at 750°C in hydrogen atmosphere, as a consequence that a voltage degradation rate of 1.7%/kh has been measured.
Performance Improvement of an Inhomogeneous Cathode by Infiltration

The performance of solid oxide fuel cells (SOFCs) is considerably influenced by the microstructure and chemical composition of cathode materials. Porous La$_{0.85}$Sr$_{0.15}$FeO$_3$–Ce$_{0.9}$Gd$_{0.1}$O$_2$ composite electrodes were infiltrated by La$_{0.6}$Sr$_{0.4}$CoO$_3$ and La$_{0.6}$Sr$_{0.4}$FeO$_3$. The effects of infiltration loading, calcination temperature of infiltrated material and co-infiltration of LSC and LSF were investigated using electrochemical impedance measurement, microstructural analysis, and high-temperature X-ray diffraction (HT-XRD). A symmetrical cell two-electrode configuration was used to examine the electrochemical performance of the electrodes. The electrochemical results revealed that the polarization resistance of the cathodes significantly was decreased by infiltration from 2.59 to 0.034 Ω cm$^2$ measured at 670 °C. The best electrode performance was achieved at a calcination temperature of 770 °C. It was also found that infiltration of LSC improved the stability of the electrodes during 145 h of testing at 620 °C in air at open circuit voltage (OCV).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, University of Tehran
Authors: Seyed-Vakili, S. V. (Ekstern), Graves, C. R. (Intern), Babaei, A. (Ekstern), Heshmati-Manesh, S. (Ekstern), Mogensen, M. B. (Intern)
Pages: 108-114
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 1
ISSN (Print): 1815-6846
Ratings:
An electrochemical reactor can be used to purify flue gasses. Such a reactor can be a multilayer structure consisting of alternating layers of porous electrodes and electrolytes (a porous cell stack). In this work optimization of such a unit has been done by changing the pore former composition and the electrode powder pre-treatment. The effect on permeability, mechanical strength and electrochemical behavior was studied in this work. The effects were evaluated by measuring the pressure difference over the samples in relation to the flow through the sample, by the ball on ring method and by electrochemical impedance spectroscopy in air at temperatures between 300 and 450 °C. The resulting structures were...
also evaluated with scanning electron microscopy. The work showed a dependence on the pore former composition and electrode powder pre-treatment resulting in variations in porosity, strength and flow resistance. A higher porosity gives a lower backpressure. The electrochemical performance shows that both thickness and amount of pore former in the electrolyte is important, but almost no dependence of electrode composition on the polarization resistances within the tested compositions.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors

**Authors:** Andersen, K. B. (Intern), Charlas, B. (Intern), Stamate, E. (Intern), Kammer Hansen, K. (Intern)

**Number of pages:** 22

**Publication date:** 2017

**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Heliyon

**Volume:** 3

**Article number:** e00371

**ISSN (Print):** 2405-8440

**Chemical engineering, Materials science**

**Electronic versions:**

**DOI:** 10.1016/j.heliyon.2017.e00371

**Source:** FindIt

**Source-ID:** 2373600545

**Publication:** Research - peer-review › Journal article – Annual report year: 2017

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**Phonon thermal conductivity of scandium nitride for thermoelectrics from first-principles calculations and thin-film growth**

The knowledge of lattice thermal conductivity of materials under realistic conditions is vitally important since many modern technologies require either high or low thermal conductivity. Here, we propose a theoretical model for determining lattice thermal conductivity, which takes into account the effect of microstructure. It is based on *ab initio* description that includes the temperature dependence of the interatomic force constants and treats anharmonic lattice vibrations. We choose ScN as a model system, comparing the computational predictions to the experimental data by time-domain thermoreflectance. Our experimental results show a trend of reduction in lattice thermal conductivity with decreasing domain size predicted by the theoretical model. These results suggest a possibility to control thermal conductivity by microstructural tailoring and provide a predictive tool for the effect of the microstructure on the lattice thermal conductivity of materials based on *ab initio* calculations.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Ceramic Engineering & Science, National University of Singapore, Linköping University

**Authors:** Kerdsongpanya, S. (Ekstern), Hellman, O. (Ekstern), Sun, B. (Ekstern), Koh, Y. K. (Ekstern), Lu, J. (Ekstern), Van Nong, N. (Intern), Simak, S. I. (Ekstern), Alling, B. (Ekstern), Eklund, P. (Ekstern)

**Number of pages:** 6

**Publication date:** 2017

**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Physical Review B

**Volume:** 96

**Issue number:** 19

**ISSN (Print):** 2469-9950

**Ratings:**

**Web of Science (2017):** Indexed yes

**BFI (2016):** BFI-level 2

**Scopus rating (2016):** CiteScore 3.16

**Web of Science (2016):** Indexed yes

**BFI (2015):** BFI-level 2
Potential- and Rate-Determining Step for Oxygen Reduction on Pt(111)

Using density functional theory calculations, we study reaction thermodynamics and kinetics for the oxygen reduction reaction (ORR) on surface coverages that develop in the 0 – 1.0 V potential range on Pt(111), with special emphasis on
the role of water. At low potentials, water affects adsorption energies of hydrophilic *O2 and *OOH intermediates but
displays a limited effect on the transition state energies for their dissociation. We calculate the O2 and OOH adsorption
and dissociation free energies at most stable surfaces in the investigated potential range and arrive at two important
conclusions 1) the ORR proceeds through the associative reaction mechanism in the diffusion and the mixed kinetic-
diffusion region and 2) moderate O2 and OOH activation energies support the notion that the reaction is predominantly
controlled by the rate prefactor. We associate the rate prefactor with the probability for an O2 molecule to replace a water
molecule on hydrophilic (OH - H2O covered) surfaces, and the inability of O2 to adsorb and dissociate on hydrophobic
(O covered) surfaces that develop at higher potentials. Finally, in light of new results, we discuss activities of Pt alloys that
lie close to the top of the volcano.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern), Vegge, T. (Intern)
Pages: 26785–26793
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry C
Volume: 121
Issue number: 48
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.856 SNIP 1.033
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Potential for dynamic pricing in district heating systems in Denmark and Finland

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalto University
Authors: Dominkovic, D. F. (Intern), Wahlroos, M. (Ekstern), Syri, S. (Ekstern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Main Research Area: Technical/natural sciences

Relations
Projects:
Potential for dynamic pricing in district heating systems in Denmark and Finland
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Efficiently utilizing energy that is currently being wasted can significantly increase energy efficiency of the system, as well as reduce the carbon footprint. In hot climates with large cooling demands, excess waste heat can be utilized via absorption chillers to generate cold. Moreover, cold from liquefied natural gas gasification process can further provide energy source for meeting the cold demand. In order to connect the large sources of waste heat and cold energy with customers demanding the cold, a significant investment in district cooling grid is a necessity. In order to deal with the mentioned issue, an existing energy balance model was complemented with Matlab algorithms in order to model the whole energy system, including the detailed representation of the district cooling grid. Singapore was chosen for a case study and several different scenarios were developed for the year 2050, with the main indicators being total primary energy supply, total CO2 emissions and total socio-economic costs. The most beneficial scenario for the year 2050 had 19.5% lower primary energy demand, 38.4% lower total socio-economic costs and 41.5% lower CO2 emissions compared to the business-as-usual scenario for the year 2050, although significant investment in the district cooling grid was included in the calculations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Nanyang Technological University, University of Zagreb
Authors: Dominkovic, D. F. (Intern), Rashid, K. A. B. A. (Ekstern), Romagnoli, A. (Ekstern), Pedersen, A. S. (Intern), Leong, K. C. (Ekstern), Krajačić, G. (Ekstern), Duić, N. (Ekstern)
Pages: 49-61
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 208
Potential Of Waste Heat And Waste Cold Energy Recovery In Singapore For District Cooling Applications: Impacts On Energy System

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Nanyang Technological University, IMechE
Authors: Dominkovic, D. F. (Intern), Romagnoli, A. (Ekstern), Fox, T. (Ekstern), Pedersen, A. S. (Intern)
Number of pages: 2
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 40th IAEE International Conference - Extended abstracts : Meeting the Energy Demands of Emerging Economies
Publisher: IAEE
Main Research Area: Technical/natural sciences
Conference: 40th Annual IAEE International Conference, Singapore, Singapore, 18/06/2017 - 18/06/2017
Electronic versions:
Extended_Abstract_Potential_of_waste_heat_and_waste_cold_energy_recovery_in_Singapore_for_district_cooling_applications.pdf
Links:
https://www.iaee.org/proceedings/article/14390
Source: PublicationPreSubmission
Source-ID: 139631753
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Printed organic smart devices characterized by nonlinear optical
In this study, we demonstrate that nonlinear optical microscopy is a promising technique to characterize organic printed electronics. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. First, we show that the different nonlinear optical signals can be used to discriminate between the polymer semiconductor material and embedded metal nanoparticles which constitute the electrode in a real device. Next we demonstrate that the TPPL quenches when applying a current between source and drain; this decrease can be used to determine the electrical characteristic of the device [1]. Finally, we show that the TPPL increases with higher temperature in the 20 - 120 °C range, closely following the supported current characteristics of the semiconductor. With this technique, we can recognize different nanomaterials and we propose that the TPPL is a good indicator to map and monitor the charge carrier density and the molecular packing of the printed polymer material. Importantly, simple calculations based on the signal levels, suggest that this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Institut de Ciències Fotòniques, Catalan Institution for Research and Advanced Studies
Authors: Pastorelli, F. (Intern), Accanto, N. (Ekstern), Jørgensen, M. (Intern), van Hulst, N. F. (Ekstern)
Pages: 38
Publication date: 2017

Host publication information
Title of host publication: PLASMONICA 2017: Book of Abstracts
Article number: T19
Main Research Area: Technical/natural sciences
Workshop: 5th International Workshop on Plasmonics (PLASMONICA 2017), Lecce, Italy, 05/07/2017 - 05/07/2017
Electronic versions:
Links:
http://www.plasmonica2017.it/
Source: PublicationPreSubmission
Source-ID: 134441400
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Printed organic smart devices characterized by ultra-short laser pulses
Resume: In this study, we demonstrate that nonlinear optical microscopy is a promising technique to characterize organic printed electronics. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. First, we show that the different nonlinear optical signals can be used to discriminate between the polymer semiconductor material and embedded nanoparticles which constitute the electrode in a real device. Next we demonstrate that the TPPL quenches when applying a current between source and drain; this decrease can be used to determine the electrical characteristic of the device. Finally, we show that the TPPL increases with higher temperature in the 20 - 120 °C range, closely following the supported current characteristics of the semiconductor. We propose that the TPPL is a good indicator to map and monitor the charge carrier density and the molecular packing of the printed polymer material. Importantly, simple calculations based on the signal levels, suggest that this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences

Probing phosphoric acid redistribution and anion migration in polybenzimidazole membranes
Micro platinum electrodes embedded in a laminated phosphoric acid doped polybenzimidazole membrane are employed to monitor the acid migration during hydrogen pump mode operation. Upon application of a constant current, an immediate ohmic resistance decrease of the membrane near the anode is observed, accompanied by a corresponding increase near the cathode side. This is a direct evidence of migration of the acid anions via the vehicle conducting mechanism, resulting in an accumulation of acid at the anode side and depletion at the cathode side. Both resistances reach a steady state value after a prolonged period of measurement, apparently balanced by the back diffusion of the acid molecules. The phenomenon is magnified at higher current densities and with increased thickness of the overall membrane, which is of significance in quantitative understanding of the proton conductivity mechanism e.g. for determination of the anionic transference number. The finding provides a technique to monitor the acid redistribution within the membrane as a basis for an engineering solution to address the long-term durability of fuel cells built around phosphoric acid doped polymer membranes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Becker, H. (Intern), Cleemann, L. N. (Intern), Aili, D. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Pages: 21-24
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemistry Communications
Volume: 82
ISSN (Print): 1388-2481
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.53 SJR 1.618 SNIP 1.076
Production and Reliability Oriented SOFC Cell and Stack Design

General information
State: Published

Original language: English
Phosphoric acid, Polybenzimidazole, Transference number, Vehicle mechanism, Migration, High temperature polymer electrolyte fuel cells
DOIs:
10.1016/j.elecom.2017.07.005
Source: PublicationPreSubmission
Source-ID: 134228917
Publication: Research - peer-review › Journal article – Annual report year: 2017
Production and Reliability Oriented SOFC Cell and Stack Design

The paper presents an innovative development methodology for a production and reliability oriented SOFC cell and stack design aiming at improving the stacks robustness, manufacturability, efficiency and cost. Multi-physics models allowed a probabilistic approach to consider statistical variations in production, material and operating parameters for the optimization phase. A methodology for 3D description of spatial distribution of material properties based on a random field models was developed and validated by experiments. Homogenized material models on multiple levels of the SOFC stack were established. The probabilistic models were related to the experimentally obtained properties of base materials to establish a statistical relationship between the material properties and the most relevant load effects. Software algorithms for meta models that allow the detection of relationships between input and output parameters and to perform a sensitivity analysis were developed and implemented. The capabilities of the methodology is illustrated on two practical cases.

General information

State: Published
Pages: 2231-2249
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: ECS Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Progress of SOFC/SOEC Development at DTU Energy: From Materials to Systems

DTU Energy has over the past 20 years had a very substantial effort on SOFC/SOEC development. The current project volume corresponds to ~40 man years per year. Activities span over a broad range in the value chain, from materials to cells, stacks and analyses at energy system level. In addition to that, research areas comprise ceramic processing methods, micro-structural analysis, electrochemical characterization, and modelling. Among recent highlights are electrode and cell developments, including metal supported cells, stack development durability studies under realistic operation conditions and stack operation at high pressure.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Hagen, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 9
Pages: 145-153
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Pulsed Laser Deposition of $\text{YBa}_2\text{Cu}_3\text{O}_x$ with Scanning Beam: Target to Substrate Composition Transfer and Film Structure

Pulsed laser deposition is often considered a process providing congruent transfer of target composition to the growing film. In fact, many different processes affect compositional preservation, starting from incongruent target ablation, to scattering on the way to the substrate, and to processes of the film formation on the substrate surface. We developed a pulsed laser deposition process trying to minimize the compositional deviations due to the scattering by the ambient gas by applying laser beam scanning across the target surface and substitution of oxygen with argon in the chamber during deposition. Transfer of elemental composition of $\text{YBa}_2\text{Cu}_3\text{O}_7$ targets with compositions varying from stoichiometric 1/2/3 ratio was tested by deposition of thin films in conditions optimal for high-temperature superconductor formation. Despite all measures, the films still show Ba,Y enrichment due to different efficiencies of scattering on the ambient gas. The Y part in the film followed well the composition of the target, but the Ba enrichment was almost constant for most of the studied target compositions, implying a crucial role of the film growth processes. The $\text{YBa}_2\text{Cu}_3\text{O}_x$ (YBCO) films show a layered structure, with increased density of defects in the topmost layer. We suppose this is due to expelling of the excess Ba into the top layer with formation of a quasi-liquid layer promoting formation of a high-density YBCO film.

General information
State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Mozhaev, P. (Intern), Khoryushin, A. (Intern), Mozhaeva, J. (Intern), Grivel, J. (Intern), Hansen, J. O. B. (Ekstern), Jacobsen, C. S. (Intern)
Number of pages: 28
Pages: 1-28
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Superconductivity and Novel Magnetism
ISSN (Print): 1557-1939
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.91 SJR 0.34 SNIP 0.546
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.325 SNIP 0.556 CiteScore 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.384 SNIP 0.637 CiteScore 0.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.326 SNIP 0.666 CiteScore 0.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.42 SNIP 0.51 CiteScore 0.64
Quality Assurance of Solid Oxide Fuel Cell (SOFC) and Electrolyser (SOEC) Stacks

In the EU-funded project “Solid oxide cell and stack testing and quality assurance” (SOCTESQA) standardized and industry wide test modules and programs for high temperature solid oxide cells and stacks are being developed. These test procedures can be applied for the fuel cell (SOFC), the electrolysis (SOEC) and in the combined SOFC/SOEC mode. In order to optimize the test modules the project partners have tested identical SOC stacks with the same test programs in several testing campaigns. Altogether 10 pre-normative test modules were developed: Start-up, current-voltage characteristics, electrochemical impedance spectroscopy, reactant utilization, reactant gas composition, temperature sensitivity, operation at constant current, operation at varying current, thermal cycling and shut-down. The test modules were validated by comparing the results in terms of repeatability of the different testing campaigns and in terms of reproducibility among the different partners. Moreover, the results are discussed in context to the test input parameters.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, German Aerospace Center (DLR), Grenoble-Alpes University, Italian National Agency for New Technologies, European Commission Joint Research Centre Institute, European Institute for Energy Research, Nanyang Technological University
Authors: Lang, M. (Ekstern), Auer, C. (Ekstern), Couturier, K. (Ekstern), Sun, X. (Intern), McPhail, S. J. (Ekstern), Malkow, T. (Ekstern), Fu, Q. (Ekstern), Liu, Q. (Ekstern)
Number of pages: 10
Pages: 2077-2086
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
Quantification of solar cell failure signatures based on statistical analysis of electroluminescence images

We propose a method to identify and quantify the extent of solar cell cracks, shunting, or damaged cell interconnects, present in crystalline silicon photovoltaic (PV) modules by statistical analysis of the electroluminescence (EL) intensity distributions of individual cells within the module. From the EL intensity distributions (ELID) of each cell, we calculated summary statistics such as standard deviation, median, skewness and kurtosis, and analyzed how they correlate with the type of the solar cell degradation.

We found that the dispersion of the ELID increases with the size and severity of the solar cell cracks, correlating with an increase in standard deviation and decrease in kurtosis. For shunted cells, we found that the ELID median is strongly correlated with the extent of cell shunting. Last, cells with damaged interconnect ribbons show current crowding and increased series resistance regions, characterized by increased dispersion and skewness of the ELID. These cell-level diagnostic parameters can be used to quantify the level of mismatch between the solar cells in the module, which can represent the extent of the module degradation, due to transportation, installation, or field operation. The method can be easily automated for quality control by module manufacturers or installers, or can be used as a diagnostic tool by plant operators and diagnostic service providers.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Aalborg University, National Renewable Energy Laboratory
Authors: Spataru, S. (Ekstern), Parikh, H. (Ekstern), Benatto, G. A. D. R. (Intern), Hacke, P. (Ekstern), Sera, D. (Ekstern), Poulsen, P. B. (Intern)
Pages: 1466-1472
Publication date: 2017

Host publication information
Title of host publication: Proceedings of 33rd European Photovoltaic Solar Energy Conference and Exhibition
Main Research Area: Technical/natural sciences
Conference: 33rd European Photovoltaic Solar Energy Conference and Exhibition
, Amsterdam, Netherlands, 25/09/2017 - 25/09/2017
Radical production efficiency and electrical characteristics of a coplanar barrier discharge built by multilayer ceramic technology

The present study investigated the electrical characteristics and radical production efficiency of a coplanar barrier discharge (CBD) device manufactured by Kyocera by multilayer ceramic technology. The device consisted of a number of linear electrodes with electrode and gap widths of 0.75 mm, immersed into a ceramic dielectric barrier. A closed flow-through system necessary for the measurements was prepared by placing a quartz plate at a height of 3 mm from the ceramic barrier. The production of nitrogen radicals was determined from the removal of a trace amount of NO in pure N2 gas, while the production of oxygen radicals was determined by ozone production in pure O2 or synthetic air. The production efficiency of N and O radicals and NO oxidation in synthetic air was comparable with the efficiency of a volume barrier discharge device. The power density per unit of surface area of the CBD device was more than two times larger than that of a similar volume barrier discharge setup, which makes the CBD device a compact alternative for gas treatment. The production of ozone and different nitrogen oxides was also evaluated for the open system of the CBD which is usable for surface treatment. The ozone concentration of this system was nearly independent from the input power, while the concentration of nitrogen oxides increased with input power. The open system of the CBD was additionally tested for the treatment of a silicon surface. An increase of applied power decreased the time required to reduce the water contact angle below 10 degrees but also started to have an impact on the surface roughness.
Reduction of the thermal conductivity of the thermoelectric material ScN by Nb alloying

ScN-rich (Sc,Nb)N solid solution thin films have been studied, motivated by the promising thermoelectric properties of ScN-based materials. Cubic Sc\(_{1-x}\)Nb\(_x\)N films for 0 ≤ x ≤ 0.25 were epitaxially grown by DC reactive magnetron sputtering on a c-plane sapphire substrate and oriented along the (111) orientation. The crystal structure, morphology, thermal conductivity, and thermoelectric and electrical properties were investigated. The ScN reference film exhibited a Seebeck coefficient of −45 μV/K and a power factor of 6 × 10\(^{-4}\) W/m K\(^2\) at 750 K. Estimated from room temperature Hall measurements, all samples exhibit a high carrier density of the order of 10\(^{21}\) cm\(^{-3}\). Inclusion of heavy transition metals into ScN enables the reduction in thermal conductivity by an increase in phonon scattering. The Nb inserted ScN thin films exhibited a thermal conductivity lower than the value of the ScN reference (10.5 W m\(^{-1}\) K\(^{-1}\)) down to a minimum value of 2.2 W m\(^{-1}\) K\(^{-1}\). Insertion of Nb into ScN thus resulted in a reduction in thermal conductivity by a factor of ∼5 due to the mass contrast in ScN, which increases the phonon scattering in the material.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Linköping University, Sorbonne Universités, Indian Institute of Technology Mandi
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences
Relation Between Ni Particle Shape Change and Ni Migration in Ni–YSZ Electrodes – a Hypothesis

This paper deals with degradation mechanisms of Ni–YSZ electrodes for solid oxide cells, mainly solid oxide electrolysis cells (SOECs), but also to some extent solid oxide fuel cells (SOFCs). Analysis of literature data reveals that several apparently different and even in one case apparently contradicting degradation phenomena are a consequence of interplay between loss of contact between the Ni–YSZ (and Ni–Ni particles) in the active fine-structured composite fuel electrode layer and migration of Ni via weakly oxidized Ni hydroxide species. A hypothesis that unravels the apparent contradiction and explains qualitatively the phenomena is presented, and as a side effect, light has been shed on a degradation phenomenon in solid oxide fuel cells (SOFCs) that has been observed during a decade.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Mogensen, M. B. (Intern), Hauch, A. (Intern), Sun, X. (Intern), Chen, M. (Intern), Tao, Y. (Intern), Ebbesen, S. D. (Intern), Hansen, K. V. (Intern), Hendriksen, P. V. (Intern)
Pages: 434-441
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Fuel Cells
Volume: 17
Issue number: 4
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.699 SNIP 0.787 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.629 SNIP 0.816 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.841 SNIP 0.848 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.25 SNIP 1.008 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Releasing cation diffusion in self-limited nanocrystalline defective ceria thin films

Acceptor-doped nanocrystalline cerium oxide thin films are mechanically constrained nano-domains, with film/substrate interfacial strain and chemical doping deadlock mass diffusion. In contrast, in this paper we show that chemical elements result in highly unstable thin films under chemical reduction, with unexpected diffusion-driven effects such as fast migration of grain boundaries, porosity nucleation, and interdiffusion at low temperatures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Electrofunctional materials, Chinese Academy of Sciences
Authors: Esposito, V. (Intern), Ni, D. W. (Ekstern), Gualandris, F. (Intern), Pryds, N. (Intern)
Pages: 13784-13788
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: R S C Advances
Volume: 7
Issue number: 23
ISSN (Print): 2046-2069
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Reply to *"Comment on 'Performance of Halbach magnet with finite coercivity'"

We reply to Dr. Xu’s comment on our paper ‘Performance of Halbach magnet arrays with finite coercivity’ (JMMM 407 (2016), 369-376). Contrary to Dr. Xu’s objections we show that the procedure employed by us correctly accounts for the shape effects of the magnet elements. We show that the partial differential equation for the magnetic vector potential, derived from the Maxwell equations, incorporates all shape effects. On the other hand, the local constitutive relations express a point-wise link between, e.g., magnetic field and magnetic flux density, and are as such independent of geometry. We confirm that the results of our computations are perfectly consistent with the constitutive relation which is assumed as starting point.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Pages: 386-389
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Magnetism and Magnetic Materials
Volume: 429
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
Understanding the interaction between adsorbants and metal surfaces has led to descriptors for bindings and catalysis which have a major impact on the design of metal catalysts. On semiconductor oxides, these understandings are still lacking. We show an important elementin understanding binding on semiconductors. We propose here a correlation between the cooperative interaction energy, i.e., the energy difference between the adsorption energies of coadsorbed electron donor–acceptor pair and isolated fragments and the band gap of the clean oxide surface. We demonstrate this effect for a number of oxides and donor–acceptor pairs and explain it with the shift in the Fermi level before and after the adsorption. The conclusion is that the adsorption of acceptor–donor pairs is considerably more favorable compared to unpaired fragments,and this energy difference is approximately equal to the value of the band gap. The implications of this understanding in relation to the improvement and discovery of novel catalysts on the band gap oxides are also discussed.
Scaling up aqueous processing of A-site deficient strontium titanate for SOFC anode supports

All ceramic anode supported half cells of technically relevant scale were fabricated in this study, using a novel strontium titanate anode material. The use of this material would be highly advantageous in solid oxide fuel cells due to its redox tolerance and resistance to coking and sulphur poisoning. Successful fabrication was possible through aqueous tape casting of both anode support and electrolyte layers and subsequent lamination. Screen printing of electrolyte layers onto green anode tapes was also attempted but resulted in cracked electrolyte layers upon firing. Microstructural, electrical and mechanical properties of anode supports and half cells will be discussed. The use of two different commercial titanate powders with nominal identical, but in reality different stoichiometries, strongly affect electrical and mechanical properties. Careful consideration of such variations between powder suppliers, and batches of the same supplier, is critical for the successful implementation of ceramic anode supported solid oxide fuel cells.
Scavenging of oxygen vacancies at modulation-doped oxide interfaces: Evidence from oxygen isotope tracing

The introduction of manganite buffer layers, La\textsubscript{7/8}Sr\textsubscript{1/8}MnO\textsubscript{3} (LSMO) in particular, at the metallic interface between SrTiO\textsubscript{3} (STO) and another band insulator suppresses the carrier density of the interfacial two-dimensional electron gas (2DEG) and improves significantly the electron mobility. However, the mechanisms underlying the extreme mobility enhancement remain elusive. Herein, we used 18O isotope exchanged SrTi\textsubscript{18}O\textsubscript{3} as substrates to create 2DEG at room temperature with and without the LSMO buffer layer. By mapping the oxygen profile across the interface between STO\textsubscript{18} and disordered LaAlO\textsubscript{3} or yttria-stabilized zirconia (YSZ), we provide unambiguous evidence that redox reactions occur at oxide interfaces even grown at room temperature. Moreover, the manganite buffer layer not only suppresses the carrier density but also strongly suppresses the oxygen exchange dynamics of the STO substrate, which likely prevents the reduction of STO during the formation of the 2DEG. The underlying mechanism on the enhanced electron mobility at buffered oxide interfaces is also discussed.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, ETH Zurich, Paul Scherrer Institut
Authors: Chen, Y. (Intern), Döbeli, M. (Ekstern), Pomjakushina, E. (Ekstern), Gan, Y. (Intern), Pryds, N. (Intern), Lippert, T. (Ekstern)
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Physical Review Materials
Volume: 1
Issue number: 5
Article number: 052002
ISSN (Print): 2475-9953
Original language: English
Electronic versions:
  - [Paper_Yunzhong_Scavenging_of_oxygen_vacancies_revised_final_001_revised_002_.pdf](#)
DOIs:
  - 10.1103/PhysRevMaterials.1.052002
Secondary creep of porous metal supports for solid oxide fuel cells by a CDM approach

The creep behaviour of porous iron-chromium alloy used in solid oxide fuel cells (SOFCs) becomes relevant under SOFC operating temperatures. In this paper, the secondary creep stage of infiltrated and non-infiltrated porous metal supports (MS) was investigated and theoretically modelled by a continuum damage mechanics (CDM) approach. The behaviour of the porous metal support, in the range from 1 to 17 MPa and temperatures between 650 and 700°C, was combined and compared with data from literature of Crofer® 22 APU, taken as zero porosity reference material. The variation of the elastic modulus as function of temperature, determined by the high temperature impulse excitation technique, was directly used to account for the porosity and the related effective stress acting during the creep tests. The proposed creep rate formulation was used to extend the Crofer® 22 APU Monkman-Grant diagram in the viscous creep regime. The influence of oxide scale formation on creep behaviour of the porous MS was assessed by comparing the creep data of pre-oxidised samples tested in reducing atmosphere.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Naples Federico II
Authors: Esposito, L. (Ekstern), Boccaccini, D. N. (Intern), Pucillo, G. P. (Ekstern), Frandsen, H. L. (Intern)
Pages: 155-161
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 691
ISSN (Print): 0921-5093
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.666 SNIP 1.832
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.78 SNIP 1.849 CiteScore 3.01
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.285 SNIP 2.617 CiteScore 3.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.879 SNIP 2.231 CiteScore 2.86
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.737 SNIP 2.351 CiteScore 2.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.741 SNIP 2.406 CiteScore 2.59
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.702 SNIP 2.086
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.551 SNIP 1.74
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.678 SNIP 1.847
Web of Science (2008): Indexed yes
Sliding-wear resistance of pure near fully-dense B4C under lubrication with water, diesel fuel, and paraffin oil

The sliding-wear resistance of pure near fully-dense B₄C is investigated, and the wear mode/mechanisms identified, under lubrication with water, diesel fuel, and paraffin oil. It is found that the wear is mild in the three cases, with specific wear rates (SWRs) of $10^{-16}$–$10^{-17}$ m³/N m. Nonetheless, the wear resistance of the B₄C ceramic is one order of magnitude greater under oil lubrication ($10^{16}$ N/m²) than under water lubrication ($10^{15}$ N/m²), and twice as great for the specific case of paraffin oil than diesel fuel, attributable to the lubricant's viscosity. It is also found that the wear mode is always abrasion, and that the wear mechanisms are plastic deformation and localized fracture with grain pullout. However, in agreement with the macro-wear data, the severity of the wear damage is lower under lubrication with paraffin oil, followed by diesel fuel, and lastly water. Finally, microstructural considerations are discussed with a view to enhancing the sliding-wear resistance of B₄C triboceramics.
Biogas is a valuable energy source and will be available in future in systems relying on renewables. It is an attractive fuel for solid oxide fuel cells (SOFC), which are able to utilize the carbon contained in the biogas and which produce electricity with high efficiency. In the current paper, state-of-the-art SOFCs were studied regarding performance and durability in relation to biogas as fuel and considering important contaminants, specifically sulfur. First, the catalytic behavior in relevant synthetic biogas mixtures was studied and the potential of dry reforming was demonstrated. Successful long term operation of an SOFC under both, conditions of steam and dry reforming, i.e., addition of steam or CO2 to avoid carbon formation was shown. For the steam reforming case a remarkable period of 3,500 h, hereof 3,000 h in the presence of H2S was achieved. Finally, a real biogas from a landfill gas unit was used as fuel. The concept of dry reforming was realized. The SOFC was successfully operated with and in one case even without a specific gas cleaning unit.
Solder free joining as a highly effective method for making contact between thermoelectric materials and metallic electrodes

Quality of joining and interfacial evolution behavior play a critical role in the performance and reliability of thermoelectric (TE) devices. In this study, different joining methods using Zn−2AlZn−2Al solder alloy (1) and solder-free joining with microlayers of Ti and Cr as interconnecting agents (2) were systematically investigated and demonstrated on the low-cost ZnSb TE system. ZnSb material, which was chosen to bond with Ag and Ni metallic electrodes, exhibited a maximum zT value of 0.8 at 400°C. With the joining method (1), Zn from the Zn−2AlZn−2Al solder was found to diffuse/react with both Ag and Ni electrodes, and penetrate into ZnSb legs. SEM-EDX analysis recorded a significant excess of Zn in the ZnSb leg after joining. We found that, using microlayers of Ti and Cr as interconnecting agent, a very good interfacial contact was obtained, and the starting composition of ZnSb legs was preserved. The interfacial contact of ZnSb/Cr/NiZnSb/Cr/Ni was found to be stable after heat treatment at 400°C for 30 h, suggesting solder-free joining as an effective method for reliable contacts in TE devices in the medium temperature region (200°C−400°C).

Spatially resolved modelling of inhomogeneous materials with a first order magnetic phase transition

We present a numerical model that can simulate a magnetocaloric sample on the grain size level, including magnetostatics, heat transfer, local hysteresis and spatial variation of stoichiometry expressed as a variation in Curie temperature. Grain structure of a sample is realised as a number of regions each having a uniform and defined through a Voronoi-map. We show that demagnetising effects, caused by a finite sample size, and spatial variation in can account for the previously experimentally observed 'virgin' effects in the adiabatic temperature change and isothermal entropy change, respectively and first order reversal effect as a function of temperature. We conclude that even a very little variation in local stoichiometry of less than a percent, corresponding to a standard deviation in of for has a significant impact on the overall properties and history dependence of a sample.
First order phase change, Magnetocaloric, Hysteresis, Model

DOIs:
10.1088/1361-6463/aa86e2
Spinel-based coatings for metal supported solid oxide fuel cells

Metal supports and metal supported half cells developed at DTU are used for the study of a solution infiltration approach to form protective coatings on porous metal scaffolds. The metal particles in the anode layer, and sometimes even in the support may undergo oxidation in realistic operating conditions leading to severe cell degradation. Here, a controlled oxidation of the porous metal substrate and infiltration of Mn and/or Ce nitrate solutions are applied for in situ formation of protective coatings. Our approach consists of scavenging the FeCr oxides formed during the controlled oxidation into a continuous and well adhered coating. The effectiveness of coatings is the result of composition and structure, but also of the microstructure and surface characteristics of the metal scaffolds.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, University of St Andrews
Pages: 232-244
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Research Bulletin
Volume: 89
ISSN (Print): 0025-5408
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.71 SNIP 0.855 CiteScore 2.39
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.733 SNIP 0.976 CiteScore 2.42
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.774 SNIP 1.051 CiteScore 2.47
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.712 SNIP 0.993 CiteScore 2.11
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.825 SNIP 1.163 CiteScore 2.14
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.882 SNIP 1.228 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.979 SNIP 1.17
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.922 SNIP 1.225
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.843 SNIP 1.207
Scopus rating (2007): SJR 0.866 SNIP 1.19
Scopus rating (2006): SJR 0.811 SNIP 1.153
Spray pyrolysis of doped-ceria barrier layers for solid oxide fuel cells

Gadolinium doped ceria (Ce0.8Gd0.2O2−x-CGO) layer fabricated by spray pyrolysis is investigated as the diffusion barrier for solid oxide fuel cell. It is deposited between the La0.6Sr0.4FeO3−δ cathode and the yttria stabilized zirconia electrolyte to mitigate harmful interdiffusion of elements. The parameters of the fabrication process are linked to the measured area specific resistances of the symmetrical cells and the efficiency of the fuel cells. Results show, that application of 800 Å thick barrier effectively hinder negative reactions, while 400 Å thick layer is sufficient to prevent degradation of the Ohmic resistance.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Szymczewska, D. (Ekstern), Chrzan, A. (Ekstern), Karczewski, J. (Ekstern), Molin, S. (Intern), Jasinski, P. (Ekstern)
Pages: 168-176
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Surface and Coatings Technology
Volume: 313
ISSN (Print): 0257-8972
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.874 SNIP 1.359
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.871 SNIP 1.415 CiteScore 2.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.998 SNIP 1.681 CiteScore 2.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.057 SNIP 1.859 CiteScore 2.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.049 SNIP 1.658 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
Stability and performance of robust dual-phase \((\text{ZrO}_2)_{0.89}\text{(Y}_2\text{O}_3)_{0.01}\text{(Sc}_2\text{O}_3)_{0.10}\text{Al}_0.02\text{Zn}_0.98\text{O}_1.01)\) oxygen transport membranes

Dual-phase composite oxygen transport membranes consisting of 50 vol% \(\text{Al}_0.02\text{Zn}_0.98\text{O}_1.01\) and 50 vol% \((\text{ZrO}_2)_{0.89}\text{(Y}_2\text{O}_3)_{0.01}\text{(Sc}_2\text{O}_3)_{0.10}\) were successfully developed and tested. The applicability of the membrane in oxy-fuel power plants schemes involving direct exposure to flue gas was evaluated by exposing the membrane to gas streams containing \(\text{CO}_2\), \(\text{SO}_2\), \(\text{H}_2\text{O}\) and investigating possible reactions between the membrane material and these gases. The analyses of the exposed composites by x-ray diffraction (XRD), x-ray fluorescence (XRF), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), and Raman spectroscopy revealed excellent stability. Additionally, an electrical conductivity measurement over 900 h confirmed that the composite is stable under prolonged exposure to \(\text{CO}_2\). However, an instability of the dual-phase membrane under oxygen partial pressures below \(10^{-4}\) atm. was found. Oxygen permeation tests on a 1 mm thick self-standing membrane resulted in an oxygen flux of 0.33 ml cm\(^{-2}\) min\(^{-1}\) at 925 °C in air/N\(_2\). Stability tests in \(\text{CO}_2\) with 3 vol% \(\text{O}_2\) demonstrated the potential for the use of 10Sc1YSZ-AZO dual-phase membranes in oxy-combustion processes involving direct exposure to flue gas.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Imperial College London
Pages: 18-27
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 543
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2 SNIP 1.771 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.433 SNIP 1.935 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.452 SNIP 2.001 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.201 SNIP 1.968 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.82 SNIP 1.726 CiteScore 4.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.821
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.638 SNIP 1.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.461 SNIP 1.805
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.474 SNIP 1.578
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.812 SNIP 2.444
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.745 SNIP 1.823
Scopus rating (2004): SJR 1.559 SNIP 1.668
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.472 SNIP 1.666
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.208 SNIP 1.856
Scopus rating (2001): SJR 1.301 SNIP 1.644
Scopus rating (2000): SJR 1.104 SNIP 1.715
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.39 SNIP 1.522
Stability of V₂O₅ Supported on Titania in the Presence of Water, Bulk Oxygen Vacancies, and Adsorbed Oxygen Atoms

A catalyst consisting of vanadium oxide submonolayers supported on rutile titanium dioxide is used for a variety of reactions. One important question is the difference between the activity of monomeric clusters (having one vanadium atom) and polymeric clusters (having more than one vanadium atom). In the case of oxidative dehydrogenation of alkanes and methanol, the reaction produces water, oxygen vacancies, and hydrogen atoms bound to the surface. For this article we use density functional theory to examine how the presence of these species on the surface affects a V₂O₅ cluster, which we assume to be a representative of a polymeric species. We find that often the presence of other species on the surface can change the composition of the cluster or break it up into two monomeric clusters.
Status report on high temperature fuel cells in Poland – Recent advances and achievements
The paper presents recent advances in Poland in the field of high temperature fuel cells. The achievements in the materials development, manufacturing of advanced cells, new fabrication techniques, modified electrodes and electrolytes and applications are presented. The work of the Polish teams active in the field of solid oxide fuel cells (SOFC) and molten carbonate fuel cell (MCFC) is presented and discussed. The review is orientated towards presenting key achievements in the technology at the scale from microstructure up to a complete power system based on electrochemical fuel oxidation. National efforts are covering wide range of aspects both in the fundamental research and the applied research. The review presents the areas of (i) novel materials for SOFC including ZrO2-based electrolytes, CeO2-based electrolytes, Bi2O3-based electrolytes and proton conducting electrolytes, (ii) cathode materials including thermal shock resistant composite cathode material and silver-containing composites, (iii) anode materials, (iv) metallic interconnects for SOFC, (v) novel fabrication techniques, (vi) pilot scale SOFC, including electrolyte supported SOFC (ES-SOFC) and anode supported SOFC (AS-SOFC), (vii) metallic supported SOFC (MS-SOFC), (viii) direct carbon SOFC (DC-SOFC), (ix) selected application of SOFC, (x) advances in MCFC and their applications, (xi) advances in numerical methods for simulation and optimization of electrochemical systems.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Institute of Power Engineering
Pages: 4366-4403
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 7
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Structural evolution during calcination and sintering of a (La0.6Sr0.4)0.99CoO3-δ nanofiber prepared by electrospinning

Design of 3-dimensional metal oxide nanofibers by electrospinning is being widely explored. However, the impacts of calcination and sintering on the resulting morphology remain unknown. For the first time, (La0.6Sr0.4)0.99CoO3-δ (LSC) nanofiber, which is among the most promising electrode materials for solid oxide fuel cells, was synthesized by sol-gel electrospinning. By elevating the temperature in oxygen using in situ transmission electron microscopy, we discovered the structural transitions from nanofibers to nanotubes and then to nano-pearl strings. This facile and up-scalable method can be widely applied to design metal oxide one-dimensional nanomaterials with precise control in both geometry (nanofiber, nanotube and nano-pearl string) and surface area (by varying grain size).
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Shenzhen University
Authors: Simonsen, S. B. (Intern), Shao, J. (Ekstern), Zhang, W. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Nanotechnology
Volume: 28
Issue number: 26
Article number: 265402
ISSN (Print): 0957-4484
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.096 SNIP 0.814
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.18 SNIP 0.966 CiteScore 3.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.465 SNIP 1.258 CiteScore 3.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.585 SNIP 1.244 CiteScore 2.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.846 SNIP 1.306 CiteScore 3.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.892 SNIP 1.461 CiteScore 3.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.844 SNIP 1.259
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.819 SNIP 1.28
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.875 SNIP 1.333
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.91 SNIP 1.36
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.934 SNIP 1.378
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.925 SNIP 1.445
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.849 SNIP 1.477
Study of geometries of active magnetic regenerators for room temperature magnetocaloric refrigeration

Room temperature magnetic refrigeration has attracted substantial attention during the past decades and continuing to increase the performance of active magnetic regenerators (AMR) is of great interest. Optimizing the regenerator geometry and related operating parameters is a practical and effective way to obtain the desired cooling performance. To investigate how to choose and optimize the AMR geometry, a quantitative study is presented by simulations based on a one-dimensional (1D) numerical model. Correlations for calculating the friction factor and heat transfer coefficient are reviewed and chosen for modeling different geometries. Moreover, the simulated impacts of various parameters on the regenerator efficiency with a constant specific cooling capacity are presented. An analysis based on entropy production minimization reveals how those parameters affect the main losses occurring inside the AMR. In addition, optimum geometry and operating parameters corresponding to the highest efficiency for different geometries are presented and compared. The results show that parallel plate and micro-channel matrices show the highest theoretical efficiency, while the packed screen and packed sphere beds are possibly more practical from the application point of view.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Authors: Lei, T. (Intern), Engelbrecht, K. (Intern), Nielsen, K. K. (Intern), Veje, C. T. (Ekstern)
Number of pages: 12
Pages: 1232–1243
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 111
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.462 SNIP 1.828
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.734 SNIP 1.898 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.576 SNIP 2.206 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.516 SNIP 2.5 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Study of Operating Parameters for Accelerated Anode Degradation in SOFCs
Solid oxide fuel cell (SOFC) applications require lifetimes of several years on the system level. A big challenge is to demonstrate such exceptionally long lifetimes in ongoing R&D projects. Accelerated or compressed testing are alternative methods to obtain this. Activities in this area have been carried out without arriving at a generally accepted methodology. This is mainly due to the complexity of degradation mechanisms on the single SOFC components as function of operating parameters. In this study, we present a detailed analysis of approx. 180 durability tests regarding degradation of single SOFC components – electrolyte, cathode and anode. The main findings include a time-dependent effect on degradation rates and the domination of anode degradation for the evaluated cell types and operating conditions. Specifically, the steam content as determined by fuel inlet composition, current density and fuel utilization was identified as major parameter, more important than for example operating temperature. The obtained knowledge is adopted to identify optimal operation profiles in order to acquire accelerated testing for lifetime investigation of SOFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Ploner, A. (Intern), Hagen, A. (Intern), Hauch, A. (Intern)
Pages: 498-507
Publication date: 2017
Main Research Area: Technical/natural sciences
Subsolidus Phase Relations of the CoOx-CuO-SrO System

The subsolidus phase relations of the CoOx-CuO-SrO system were investigated in air. The samples were equilibrated at 900 °C. The pseudo-ternary section contains three stoichiometric binary oxide phases (Sr2CuO3, SrCuO2, and Sr14Cu24O41−δ) and a binary oxide solid solution: Sr6+xCo5−yCuyO15+δ (0 ≤ x ≤ 0.36). Two binary phases extend into the ternary system forming solid solutions, i.e., Sr14Cu24−xCoxO41−δ (0 ≤ x ≤ 5) and Sr6+xCo5−yCuyO15+δ (0 ≤ x ≤ 0.36, 0 ≤ y ≤ 1.0). The Sr6+xCo5O15+δ solid solution was found to undergo a phase separation into a mixture of Sr6Co5O15−δ and Sr14Co11O33 upon annealing at 600 °C. This transformation is reversible.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Grivel, J. (Intern)
Pages: 646-655
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Phase Equilibria and Diffusion
Volume: 38
Issue number: 5
ISSN (Print): 1547-7037
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.487 SNIP 0.724
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.419 SNIP 0.605 CiteScore 0.64
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.444 SNIP 0.903 CiteScore 0.73
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.355 SNIP 0.733 CiteScore 0.47
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.502 SNIP 0.758 CiteScore 0.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.4 SNIP 0.685 CiteScore 0.44
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.663
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.432 SNIP 0.837
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.504 SNIP 0.512
Scopus rating (2007): SJR 0.291 SNIP 0.532
Scopus rating (2006): SJR 0.379 SNIP 0.767
Scopus rating (2005): SJR 0.478 SNIP 0.855
Scopus rating (2004): SJR 0.456 SNIP 0.867
Scopus rating (2003): SJR 0.594 SNIP 0.727
Scopus rating (2002): SJR 0.503 SNIP 0.669
SUN HUB – ENERGY HUB FOR OUTDOOR TABLES
Solar cells integrated into products are attracting more and more attention especially due to the dramatically declining cost of solar cells. Furthermore, we are getting more dependent on portable units like mobile phones, tablets and PCs which has to be charged to be of any use. Especially on festivals where people camps for several days it can be hard to have your portable units charged. In this this work we report a solar powered hub, as an add-on to a table in the urban environment for charging mobile phones and tablets and other handheld devices through USBs, charging laptops through AC connections, providing opportunity to stream music via Bluetooth and play it from a handheld device to the table and lastly to provide LED lighting on the table during the dark hours. 3 prototypes of the system was built and tested at the Roskilde Festival 2017. Electrical logger units were built into the 3 Sun Hubs to monitor the overall energy system and the consumption of each functionality in the table.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Outsider
Authors: Poulsen, P. B. (Intern), Benatto, G. A. D. R. (Intern), Riedel, N. (Intern), Thorsteinsson, S. (Intern), Santamaria Lancia, A. A. (Intern), Symonowicz, J. K. (Intern), Retoft, K. (Ekstern), Mogensen, I. (Ekstern)
Number of pages: 4
Publication date: 2017

Host publication information
Title of host publication: Proceedings of 33rd European Photovoltaic Solar Energy Conference and Exhibition
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 139806380
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Suppressed carrier density for the patterned high mobility two-dimensional electron gas at γ-Al2O3/SrTiO3 heterointerfaces
The two-dimensional electron gas (2DEG) at the non-isostuctural interface between spinel γ-Al2O3 and perovskite SrTiO3 is featured by a record electron mobility among complex oxide interfaces in addition to a high carrier density up to the order of 10^{15} cm^{-2}. Herein, we report on the patterning of 2DEG at the γ-Al2O3/SrTiO3 interface grown at 650 °C by pulsed laser deposition using a hard mask of LaMnO3. The patterned 2DEG exhibits a critical thickness of 2 unit cells γ-Al2O3 for the occurrence of interface conductivity, similar to the unpatterned sample. However, its maximum carrier density is found to be approximately 3×10^{13} cm^{-2}, much lower than that of the unpatterned sample (∼10^{15} cm^{-2}). Remarkably, a high electron mobility of approximately 3,600 cm²V^{-1}s^{-1} was obtained at low temperatures for the patterned 2DEG at a carrier density of ∼7×10^{12} cm^{-2}, which exhibits clear Shubnikov-de Hass quantum oscillations. The patterned high-mobility 2DEG at the γ-Al2O3/SrTiO3 interface paves the way for the design and application of spinel/perovskite interfaces for high-mobility all-oxide electronic devic

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, Nanjing University
Number of pages: 4
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 111
Surface characterization of coated cathodes with lithium phosphorous oxynitride thin film for all-solid-state Li-S batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Blanchard, D. (Intern), Stamate, E. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-13
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
Surface_characterization_of_Lipon_thin_film_cathodes.pdf
Links:
http://www.sustain.dtu.dk/
Source: PublicationPreSubmission
Source-ID: 140105455
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Surface defects on the Gd$_2$Zr$_2$O$_7$ oxide films grown on textured NiW technical substrates by chemical solution method

Epitaxial growth of oxide thin films has attracted much interest because of their broad applications in various fields. In this study, we investigated the microstructure of textured Gd$_2$Zr$_2$O$_7$ films grown on (001)〈100〉 orientated NiW alloy substrates by a chemical solution deposition (CSD) method. The aging effect of precursor solution on defect formation was thoroughly investigated. A slight difference was observed between the as-obtained and aged precursor solutions with respect to the phase purity and global texture of films prepared using these solutions. However, the surface morphologies are different, i.e., some regular-shaped regions (mainly hexagonal or dodecagonal) were observed on the film prepared using the as-obtained precursor, whereas the film prepared using the aged precursor exhibits a homogeneous structure. Electron backscatter diffraction and scanning electron microscopy analyses showed that the Gd$_2$Zr$_2$O$_7$ grains present within the regular-shaped regions are polycrystalline, whereas those present in the surrounding are epitaxial. Some polycrystalline regions ranging from several micrometers to several tens of micrometers grew across the NiW grain boundaries underneath. To understand this phenomenon, the properties of the precursors and corresponding xerogel were studied by Fourier transform infrared spectroscopy and coupled thermogravimetry/differential thermal analysis. The results showed that both the solutions mainly contain small Gd[ZrO] clusters obtained by the reaction of zirconium acetylacetonate with propionic acid during the precursor synthesis. The regular-shaped regions were probably formed by large Gd[ZrO] frameworks with a metastable structure in the solution with limited aging time. This study demonstrates the importance of the precise control of chemical reaction path to enhance the stability and homogeneity of the precursors of the CSD route.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Shanghai Jiao Tong University
Authors: Zhao, Y. (Ekstern), Opata, Y. A. (Intern), Wu, W. (Ekstern), Grivel, J. (Intern)
Number of pages: 7
Pages: 58-64
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Characterization
Volume: 124
Surface-Initiated Atom Transfer Radical Polymerization from Electrospun Mats: An Alternative to Nafion

Proton exchange membranes for fuel cell applications are synthesized by surface-initiated (SI) atom transfer radical polymerization (ATRP). Poly(vinylidene fluoride-co-chlorotrifluoroethylene) is electrospun into 50 μm thick mat, which is then employed as multifunctional initiator for copper-mediated SI ATRP of 4-styrene sulfonic acid sodium salt. Fine-tuning...
of the ATRP conditions allows adjustment of the membrane's ion exchange capacity by varying the loading of the grafted ionomer. Structure and composition of the membranes are investigated by spectroscopic means and thermogravimetric analysis, respectively. The membrane morphology is probed by scanning electron microscopy. A membrane with proton conductivity as high as 100 mS cm$^{-1}$ is obtained. Long-term durability study in direct methanol fuel cells is conducted for over 1500 h demonstrating the viability of this novel facile approach.

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Energy Conversion and Storage, Bulgarian Academy of Sciences, Teknologisk Institut

Authors: Javakhishvili, I. (Intern), Dimitrov, I. (Ekstern), Tynelius, O. (Ekstern), Hales, J. H. (Ekstern), Jankova Atanasova, K. (Intern), Hvilsted, S. (Intern)

Publication date: 2017

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Macromolecular Materials & Engineering

Volume: 302

Issue number: 4

Article number: 1600410

ISSN (Print): 1438-7492

Ratings:

BFI (2018): BFI-level 1

BFI (2017): BFI-level 1

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 3.01 SJR 0.894 SNIP 0.971

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1

Scopus rating (2015): SJR 0.852 SNIP 1.097 CiteScore 2.88

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1

Scopus rating (2014): SJR 1.005 SNIP 1.309 CiteScore 2.81

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1

Scopus rating (2013): SJR 0.952 SNIP 1.244 CiteScore 2.66

ISI indexed (2013): ISI indexed yes

BFI (2012): BFI-level 1

Scopus rating (2012): SJR 0.949 SNIP 1.145 CiteScore 2.34

ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1

Scopus rating (2011): SJR 0.962 SNIP 1.055 CiteScore 2.18

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1

Scopus rating (2010): SJR 0.923 SNIP 0.917

Web of Science (2010): Indexed yes

BFI (2009): BFI-level 1

Scopus rating (2009): SJR 1.069 SNIP 0.983

BFI (2008): BFI-level 1

Scopus rating (2008): SJR 0.941 SNIP 0.941

Scopus rating (2007): SJR 0.821 SNIP 0.85

Scopus rating (2006): SJR 0.936 SNIP 1.154

Scopus rating (2005): SJR 0.941 SNIP 0.956

Scopus rating (2004): SJR 0.814 SNIP 0.928

Scopus rating (2003): SJR 0.966 SNIP 1.083

Scopus rating (2002): SJR 0.595 SNIP 0.669

Scopus rating (2001): SJR 0.596 SNIP 0.728
Synthesis of conjugated polymers with complex architecture for photovoltaic applications

A common approach to bulk heterojunction solar cells involves a “trial-and-error” approach in finding optimal kinetically unstable morphologies. An alternative approach assumes the utilization of complex polymer architectures, such as donor–acceptor block copolymers. Because of a covalent preorganization of the donor and acceptor components, these materials may form desirable morphologies at thermodynamic equilibrium. This chapter reviews synthetic approaches to such architectures and shows the first photovoltaic results.

Testing of Electrodes, Cells and Short Stacks

The present contribution describes the electrochemical testing and characterization of electrodes, cells, and short stacks. To achieve the maximum insight and results from testing of electrodes and cells, it is obviously necessary to have a good understanding of the fundamental principles of electrochemistry, but it also requires proper test geometries and set up, well-chosen operating conditions for different test purposes, correct probing of voltages and temperatures, solid knowledge on benefits and drawbacks of different characterization techniques to obtain reliable, accurate, and reproducible electrochemical measurements, and this will be the focus of this chapter. First, the important issue of understanding potential differences and measurements of potentials, which is linked to the choice of proper electrode geometries and test set up configurations for electrode and cell testing, is presented. Then probing of voltages and temperatures, choice of sealing and contacting, as well as considerations regarding the choice of operating conditions for different purposes mainly for single cell testing are outlined. Having considered optimization of test set up, geometries, and the selection of optimal operating conditions, the details of measurement of the electrochemical performance of the electrode, cell, or stack are explained. As part of this, the concept of area specific resistance (ASR) and how DC and AC methods can be used and optimized to provide not only the total ASR, but also the electrochemical characterization of specific parts (electrolyte, each electrode) in a full cell are described. Some experimental results are provided including illustrative examples of breakdown of losses in full cells and determination of their temperature and gas composition dependencies, and finally, challenging issues, such as the effects of impurities and the problem of leakage in cell testing, are discussed as well.
The Atomic Simulation Environment - A Python library for working with atoms

The Atomic Simulation Environment (ASE) is a software package written in the Python programming language with the aim of setting up, steering, and analyzing atomistic simulations. In ASE, tasks are fully scripted in Python. The powerful syntax of Python combined with the NumPy array library make it possible to perform very complex simulation tasks. For example, a sequence of calculations may be performed with the use of a simple “for-loop” construction. Calculations of energy, forces, stresses and other quantities are performed through interfaces to many external electronic structure codes or force fields using a uniform interface. On top of this calculator interface, ASE provides modules for performing many standard simulation tasks such as structure optimization, molecular dynamics, handling of constraints and performing nudged elastic band calculations.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Micro- and Nanotechnology, Theoretical Nanotechnology, Universitat de Barcelona, University of Copenhagen, Malmö University, SINTEF, Aarhus University, Brown University, University of Wisconsin-Madison, University of Warwick, Carnegie Mellon University, Purdue University, Siminn, Karlsruhe Institute of Technology KIT, ETH Zurich, University of Freiburg
Number of pages: 30
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Condensed Matter
Volume: 29
Article number: 273002
ISSN (Print): 0953-8984
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.89 SJR 0.881 SNIP 0.754
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
The Effect of Electrical Polarization on Electronic Structure in LSM Electrodes: An Operando XAS, RIXS and XES Study

The influence of electrical polarization on Mn in La$_{0.5}$Sr$_{0.5}$MnO$_{3+\delta}$ electrodes has been investigated by operando High Energy Resolved Fluorescence Detected X-Ray Absorption Near-Edge Structure (HERFD-XANES) spectroscopy, K$_\beta$ X-ray Emission Spectroscopy (XES) and Resonant Inelastic X-ray Scattering (RIXS) at the Mn K-edge. The study of polarization induced changes in the electronic properties and structure has been carried out at 500°C in 10–20% O$_2$ with electrical polarization applied in the range from −850 mV to 800 mV. Cathodic polarizations in the range −600 mV to −850
mV induced a shift in the Mn K edge energy towards lower energies. The shift is assigned to a decrease in the average Mn oxidation state, which based on Kβ XES changes from 3.4 at open circuit voltage to 3.2 at −800 mV applied potential. Furthermore, RIXS rendered pronounced changes in the population of the Mn 3d orbitals, due to filling of the Mn d-orbitals during the cathodic polarization. Overall, the study experimentally links the electrical polarization of LSM electrodes to the structural and electronic properties of Mn - these properties are expected to be of major importance for the electrocatalytic performance of LSM electrode towards the oxygen reduction reaction.
The Effect of Nano-TiC Addition on Sintered Nd-Fe-B Permanent Magnets

This paper addresses the effect of nano-TiC addition on sintered Nd-Fe-B permanent magnets. TiC nanoparticles were added to sintered Nd-Fe-B magnets with a specific aim to improve the Curie temperature and thermal stability. A standard powder metallurgy route was adopted to prepare the magnets. It was found that introducing nano-TiC prior to jet milling was effective as the nanoparticles dispersed in the final alloy, concentrating in the neodymium-rich phase of the magnets. Magnets with optimal properties were obtained with the addition of 1 wt% TiC nanoparticles. The hysteresis loop for such magnets showed an improved shape and VSM analysis a coercivity value of 1188 kA/m, a remanence value of 0.96 T and a maximum energy product of 132 kJ/m³. The maximum working point and the Curie temperature of the developed magnets were 373 K and 623 K respectively.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Wind Turbine Structures and Component Design, Tallinn University of Technology, National Institute of Chemical Physics and Biophysics
Authors: Mural, Z. (Ekstern), Kollo, L. (Ekstern), Xia, M. (Intern), Bahl, C. (Intern), Abrahamsen, A. B. (Intern), Neves Bez, H. (Intern), Link, J. (Ekstern), Veinthal, R. (Ekstern)
Number of pages: 11
Pages: 23–28
Publication date: 2017
Main Research Area: Technical/natural sciences
The effect of tapering on a magnetocaloric regenerator bed

To design a high efficiency magnetocaloric heat pump for the residential sector, we focused on the improvement of the performance of the regenerator bed. In particular, placing the regenerators circumferentially on a plane, we decided to use tapered regenerators instead of the straight channel ones. Therefore, this paper investigates the effect of the tapering of the regenerators, which exhibit better air-gap utilization. Several simulations using a 1D AMR model were run to study the performance of the tapered regenerator, and the results were compared to the case of the straight regenerator bed. Moreover, the temperature span was held fixed at 25 K, and the working temperature of the regenerator was shifted to study the sensitivity to the variation of the working conditions. This paper considers a 10-layer regenerator, with Curie
temperature ($T_C$) spacing of 2.5 K.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Dallolio, S. (Intern), Lei, T. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern)
Pages: 300-308
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Refrigeration
Volume: 84
ISSN (Print): 0140-7007
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.372 SNIP 1.786
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.569 SNIP 1.954
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.309 SNIP 1.737
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 0.841 SNIP 1.646
- Scopus rating (2006): SJR 1.5 SNIP 1.629
- Scopus rating (2005): SJR 1.409 SNIP 1.718
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.193 SNIP 1.933
- Scopus rating (2003): SJR 1.241 SNIP 1.542
- Scopus rating (2002): SJR 1.592 SNIP 1.807
- Scopus rating (2001): SJR 1.775 SNIP 1.86
The future of transportation in sustainable energy systems: Opportunities and barriers in a clean energy transition

Energy demand of a transport sector has constantly been increasing in the recent years, consuming one third of the total final energy demand in the European Union (EU) over the last decade. A transition of this sector towards sustainable one is facing many challenges in terms of suitable technology and energy resources. Especially challenging transition is envisaged for heavy-weight, long-range vehicles and airplanes. A detailed literature review was carried out in order to detect the current state of the research on clean transport sector, as well as to point out the gaps in the research. In order to calculate the resources needed for the transition towards completely renewable transport sector, four main alternatives to the current fossil fuel systems were assessed and their potential was quantified, i.e. biofuels, hydrogen, synthetic fuels (electrofuels) and electricity. Results showed that electric modes of transport have the largest benefits and should be the main aim of the transport transition. It was calculated that 72.3% of the transport energy demand on the EU level could be directly electrified by the technology existing today. For the remaining part of the transport sector a significant demand for energy resources exists, i.e. 3069 TWh of additional biomass was needed in the case of biofuels utilization scenario while 2775 TWh of electricity and 925 TWh of heat were needed in the case of renewable electrofuels produced using solid oxide electrolysis scenario.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Aalborg University, University of Zagreb
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Pedersen, A. S. (Intern), Krajačić, G. (Ekstern)
Pages: 1823-1838
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Renewable & Sustainable Energy Reviews
Volume: 82
Issue number: Part 2
ISSN (Print): 1364-0321
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 9.52 SJR 3.051 SNIP 3.454
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.999 SNIP 3.387 CiteScore 8.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.106 SNIP 3.761 CiteScore 7.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.072 SNIP 3.889 CiteScore 7.88
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.814 SNIP 3.915 CiteScore 7.24
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
The influence of carbon and oxygen on the magnetic characteristics of press-less sintered NdFeB magnets

The Pressless Process (PLP) was adopted to manufacture NdFeB sintered magnets, where the investigations on carbon and oxygen residues from heptane milling liquid media and graphite crucibles used for sintering were quantified to evaluate the influence on the magnetic characteristics. The carbon and oxygen content in the magnets produced from wet ball milling of strip cast flakes was found to be of the order 10^4 ppm and 4·10^4 ppm respectively, which resulted in soft magnetic behavior. However using jet milling the carbon and oxygen concentration were decreased by an order of magnitude resulting in coercivity of up to 829 kA/m. Thus the influence of the carbon from the graphite crucibles is small.
The La(Fe,Mn,Si)$_{13}$H$_x$ magnetic phase transition under pressure

We study the magnetocaloric metamagnetic transition in LaFe$_{11.74}$Mn$_{0.06}$Si$_{1.20}$ and LaFe$_{11.76}$Mn$_{0.06}$Si$_{1.18}$H$_{1.65}$ under hydrostatic pressure up to 1.2 GPa. For both compounds, hydrostatic pressure depresses the zero field critical
temperature. However, in detail, pressure influences the magnetic properties in different ways in the two compounds. In the dehydrogenated case the transition broadens under pressure whereas in the hydrogenated case the transition sharpens. In both cases thermal hysteresis increases under pressure, although with different trends. These observations suggest both intrinsic and extrinsic hysteretic loss brought about by the use of hydrostatic pressure. We explore the multicaloric field-pressure cycle, demonstrating that although the gain introduced by overcoming the magnetic hysteretic loss is closely countered by the loss introduced in the pressure cycle, there are significant advantages in that the temperature range of operation can be finely tuned and extended, and the magnetocaloric transition can operate in lower absolute applied fields (<0.5 T), potentially overcoming one of the most significant bottlenecks to the commercialization of this technology.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT, Imperial College London, Iowa State University
Authors: Lovell, E. (Ekstern), Bez, H. N. (Ekstern), Boldrin, D. C. (Ekstern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. (Intern), Cohen, L. F. (Ekstern)
Number of pages: 5
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 11
Issue number: 8
Article number: 1700143
ISSN (Print): 1862-6254
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.89 SJR 1.237 SNIP 1.141
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.194 SNIP 1.003 CiteScore 2.39
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.161 SNIP 0.942 CiteScore 2.19
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.16 SNIP 1.05 CiteScore 2.34
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.451 SNIP 1.283 CiteScore 2.34
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.531 SNIP 1.32 CiteScore 2.48
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.816 SNIP 1.239
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.697 SNIP 1.204
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.306 SNIP 1.101
Web of Science (2007): Indexed yes
Original language: English
Hydrostatic pressure, Hysteresis, Magnetocaloric effect, Multicaloric effect, Phase transitions
DOIs: 10.1002/pssr.201700143
Publication: Research - peer-review › Journal article – Annual report year: 2017
The maximum theoretical performance of unconcentrated solar photovoltaic and thermoelectric generator systems

The maximum efficiency for photovoltaic (PV) and thermoelectric generator (TEG) systems without concentration is investigated. Both a combined system where the TEG is mounted directly on the back of the PV and a tandem system where the incoming sunlight is split, and the short wavelength radiation is sent to the PV and the long wavelength to the TEG, are considered. An analytical model based on the Shockley-Queisser efficiency limit for PVs and the TEG figure of merit parameter $zT$ is presented. It is shown that for non-concentrated sunlight, even if the TEG operates at the Carnot efficiency and the PV performance is assumed independent of temperature, the maximum increase in efficiency is 4.5 percentage points (pp.) for the combined case and 1.8pp. for the tandem case compared to a stand alone PV. For a more realistic case with a temperature dependent PV and a realistic TEG, the gain in performance is much lower. For the combined PV and TEG system it is shown that a minimum $zT$ value is needed in order for the system to be more efficient than a stand alone PV system.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern)
Pages: 264-268
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Conversion and Management
Volume: 156
ISSN (Print): 0196-8904
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.04 SJR 2.287 SNIP 2.065
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.09 SNIP 2.092 CiteScore 5.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.854 SNIP 2.835 CiteScore 5.35
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.669 SNIP 2.558 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 2.277 CiteScore 3.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.292 SNIP 1.846 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.75
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.339 SNIP 1.797
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.508 SNIP 1.905
The promise of negative emissions

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Livermore, Arizona State University, Columbia University, University of Michigan, University of California, Colorado School of Mines
Authors: Lackner, K. S. (Ekstern), Aines, R. (Ekstern), Atkins, S. (Ekstern), Barrett, S. (Ekstern), Barteau, M. (Ekstern), Braun, R. J. (Ekstern), Brouwer, J. (Ekstern), Broecker, W. (Ekstern), Browne, J. B. (Ekstern), Graves, C. R. (Intern)
Pages: 714
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 354
Issue number: 6313
ISSN (Print): 0036-8075
Ratings:
BFI (2018): BFI-level 3
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 12.012 SNIP 8.269 CiteScore 12.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 12.305 SNIP 7.87 CiteScore 12.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 13.159 SNIP 8.124 CiteScore 12.39
ISI indexed (2012): ISI indexed yes
Thermal behavior and decomposition of cerium(III) butanoate, pentanoate and hexanoate salts upon heating in argon

The thermal behavior and decomposition of Ce-butanoate monohydrate (Ce(C$_3$H$_7$CO$_2$)$_3$·H$_2$O), Ce-pentanoate (Ce(C$_4$H$_9$CO$_2$)$_3$) and Ce-hexanoate (Ce(C$_5$H$_{11}$CO$_2$)$_3$) were studied in a flow of argon while heating at 5 °C/min. By means of several techniques such as simultaneous TG-DTA, FTIR evolved gas analysis, in-situ x-ray diffraction using a synchrotron source and hot-stage microscopy, it was found that all three compounds undergo melting transitions prior to decomposition and that decomposition involves intermediate stages including at least a Ce$_2$O(C$_n$H$_{2n+1}$CO$_2$)$_4$ intermediate (n = 3, 4 or 5 for Ce-butanoate, pentanoate or hexanoate respectively). The final decomposition product consists of CeO$_2$, which is formed through a Ce-oxycarbonate. The Ce$^{3+}$ $\rightarrow$ Ce$^{4+}$ oxidation seems to proceed via Ce$_2$O$_3$ that first results from the decomposition of the oxycarbonate phase. During the whole decomposition process, the evolved gas species consist of CO$_2$ and symmetrical ketones.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Suarez Guevara, M. J. (Intern), Yue, Z. (Intern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Bednarcik, J. (Ekstern)

Bibliographical note
The full list of 46 authors and affiliations is available in the supplementary materials.

Original language: English
DOIs: 10.1126/science.aal2432
Thermal operating window for PEDOT:PSS films and its related thermoelectric properties

The intrinsically conducting polymer PEDOT:PSS is widely used and has found high recognition due to its excellent electrical conductivity. Its potential applications cover many fields, e.g. thermoelectric energy conversion. Therefore we
compared the thermoelectric properties of pristine and DMSO treated PEDOT:PSS films at potential operating temperatures. Here we observed the electrical degradation of the film up to complete failure. Further, the thermal aging of PEDOT:PSS still lacks of understanding. It is pointed out that PEDOT:PSS films show a complex degradation mechanism which includes a morphological and a chemical part. In the range of room temperature and ∼160 °C PEDOT:PSS films follow the known exponential degradation which imposes morphological degradation, while at higher temperatures this law is not suitable to match the experimental data. Thus we extended the known exponential equation by an additional exponential degradation term which shows good agreement with the experimental data. The optical absorption spectrum indicates a loss in bipolaron and polaron charge carriers, which reflects the degradation behavior. It can be seen that changes in the optical absorption spectrum after isothermal annealing for more than 50 h occur at temperatures around 120 °C, which marks the transition from morphological to chemical degradation.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Fraunhofer Institute for Material and Beam Technology
Authors: Stepien, L. (Ekstern), Roch, A. (Ekstern), Tkachov, R. (Ekstern), Leupolt, B. (Ekstern), Han, L. (Intern), Van Nong, N. (Intern), Leyens, C. (Ekstern)
Pages: 49-54
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Synthetic Metals
Volume: 225
ISSN (Print): 0379-6779
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.675 SNIP 0.764 CiteScore 2.45
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.643 SNIP 0.75 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.711 SNIP 0.943 CiteScore 2.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.721 SNIP 0.961 CiteScore 2.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.842 SNIP 1.007 CiteScore 2.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.777 SNIP 0.916 CiteScore 2.01
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.808 SNIP 0.879
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.966 SNIP 1.083
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.074 SNIP 0.928
Scopus rating (2007): SJR 1.229 SNIP 0.991
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.92 SNIP 0.734
Web of Science (2006): Indexed yes
Thermodynamic assessment of the oxygen reduction activity in aqueous solutions

In the conventional theoretical approach, oxygen reduction reaction activities are assessed through a volcano plot using activity descriptors. The volcano plot relies on several approximations, e.g. the reaction kinetics are commonly overlooked and the interaction of hydrophilic intermediates with water is considered constant regardless of the metal surface. Herein, we demonstrate by means of density functional theory calculations that the binding energies of hydrophilic intermediates are strongly influenced by hydrogen bonding (HB) to surface water molecules. We find the HB energies of adsorbed OOH and OH on a number of active metallic (strained and non-strained Pt, Pd, Ag) and bimetallic (Pt3Ni, Pt3Co, PtCu, Pd@Pt-skin and Pt@Pd-skin) 111 surfaces to vary by up to 0.5 eV in energy. Furthermore, we show that the existence of a universal scaling line is a relative notion, contingent on how large errors in activity predictions can be tolerated. Scaling errors can be reduced substantially by partitioning data into subsets depending on the element comprising the surface layer. Finally, the activity volcano that explicitly includes HB and van der Waals interactions reproduces the right experimental trend for Pt and its alloys, but at the same time predicts Ag to be a more active catalyst than Pt. The latter result can be explained by having a fundamentally different water structure on Ag(111) than on the other metals, and the fact that reaction kinetics have been neglected in the analysis.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern)
Pages: 29381-29388
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 2017
Issue number: 19
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
Thermodynamic Ground States of Complex Oxide Heterointerfaces

The formation mechanism of 2-dimensional electron gases (2DEGs) at heterointerfaces between nominally insulating oxides is addressed with a thermodynamical approach. We provide a comprehensive analysis of the thermodynamic ground states of various 2DEG systems directly probed in high temperature equilibrium conductivity measurements. We unambiguously identify two distinct classes of oxide heterostructures: For epitaxial perovskite/perovskite heterointerfaces (LaAlO3/SrTiO3, NdGaO3/SrTiO3, and (La,Sr)(Al,Ta)O3/SrTiO3), we find the 2DEG formation being based on charge transfer into the interface, stabilized by the electric field in the space charge region. In contrast, for amorphous LaAlO3/SrTiO3 and epitaxial γ-Al2O3/SrTiO3 heterostructures, the 2DEG formation mainly relies on the formation and accumulation of oxygen vacancies. This class of 2DEG structures exhibits an unstable interface reconstruction associated with a quenched nonequilibrium state.

Thermodynamic Ground States of Complex Oxide Heterointerfaces

The formation mechanism of 2-dimensional electron gases (2DEGs) at heterointerfaces between nominally insulating oxides is addressed with a thermodynamical approach. We provide a comprehensive analysis of the thermodynamic ground states of various 2DEG systems directly probed in high temperature equilibrium conductivity measurements. We unambiguously identify two distinct classes of oxide heterostructures: For epitaxial perovskite/perovskite heterointerfaces (LaAlO3/SrTiO3, NdGaO3/SrTiO3, and (La,Sr)(Al,Ta)O3/SrTiO3), we find the 2DEG formation being based on charge transfer into the interface, stabilized by the electric field in the space charge region. In contrast, for amorphous LaAlO3/SrTiO3 and epitaxial γ-Al2O3/SrTiO3 heterostructures, the 2DEG formation mainly relies on the formation and accumulation of oxygen vacancies. This class of 2DEG structures exhibits an unstable interface reconstruction associated with a quenched nonequilibrium state.


**Thermofluid topology optimization of heat sinks**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Haertel, J. H. K. (Intern), Lei, T. (Intern), Alexandersen, J. (Intern), Engelbrecht, K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern)

**Publication information**
Journal: A C S Applied Materials and Interfaces
Volume: 9
Issue number: 1
ISSN (Print): 1944-8244
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 1.571 SNIP 0.931
- Web of Science (2010): Indexed yes
- Web of Science (2009): Indexed yes
Original language: English
2DEG, Defect-chemistry, Interface chemistry, Oxide heterointerfaces, Thermodynamics
DOI: 10.1021/acsami.6b12706
Source: FindIt
Source-ID: 2349487651
Publication: Research - peer-review › Journal article – Annual report year: 2016

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**Thermofluid topology optimization of heat sinks**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, RWTH Aachen University, Forschungs Zentrum Jülich GmbH
Authors: Gunkel, F. (Ekstern), Hoffmann-Eifert, S. (Ekstern), Heinen, R. A. (Ekstern), Christensen, D. V. (Intern), Chen, Y. (Intern), Pryds, N. (Intern), Waser, R. (Ekstern), Dittmann, R. (Ekstern)

**Publication information**
Journal: A C S Applied Materials and Interfaces
Volume: 9
Issue number: 1
ISSN (Print): 1944-8244
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 1.571 SNIP 0.931
- Web of Science (2010): Indexed yes
- Web of Science (2009): Indexed yes
Original language: English
2DEG, Defect-chemistry, Interface chemistry, Oxide heterointerfaces, Thermodynamics
DOI: 10.1021/acsami.6b12706
Source: FindIt
Source-ID: 2349487651
Publication: Research - peer-review › Journal article – Annual report year: 2016
Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Chen, M. (Intern), Sun, X. (Intern), Chatzichristodoulou, C. (Intern), Koch, S. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: Electrochemical Society, Incorporated
Article number: 287
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/287
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode
High temperature electrolysis based on solid oxide electrolysis cells (SOECs) is a promising technology for energy storage and synthetic fuel production. In recent years extensive efforts have been devoted to improving performance and durability of SOEC cells and stacks. Due to historical reasons and the convenience of doing constant current tests, (almost) all the reported SOEC tests have been galvanostatic. In this work, we report test results on two types of SOEC cells operated for electrolysis of steam in potentiostatic mode at 1.29 V. Both cells are Ni/YSZ fuel electrode supported type with different oxygen electrodes. The two cells exhibited different initial performance and different long-term degradation behavior. Detailed impedance analysis indicates that degradation happened mainly at the Ni/YSZ electrode for both cells. Large overpotential on the Ni/YSZ electrode was identified as the main cause of the degradation. Operation strategies were further proposed for electrolysis operation in potentiostatic mode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Chen, M. (Intern), Sun, X. (Intern), Chatzichristodoulou, C. (Intern), Koch, S. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Pages: 3077-3088
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
The role of CO* as a spectator in CO2 electro-reduction on RuO2
RuO2-based electrocatalysts are found to be active at low overpotential toward direct electrochemical reduction of CO2 to formic acid and methanol. RuO2 can circumvent the thermodynamic bottleneck resulting from the scaling relations observed on metallic electrocatalyst, by utilizing an alternate pathway through oxygen-coordinated intermediates. Employing density functional theory based computational electrocatalysis models we show adsorbate–adsorbate interaction effects for adsorbates and reaction intermediates on the RuO2(110) surface are large and impactful to the reaction thermodynamics. We studied binding energy amendment due to adsorbate interaction (steric and electronic) with varying coverage of CO* spectators on the catalyst surface. Implications on the reaction pathways help us rationalize differences in experimentally observed carbonaceous product mix and suppression of the hydrogen evolution reaction (HER). We show that a moderate CO* coverage (∼50%) is necessary for obtaining methanol as a product and that higher CO* coverages leads to very low overpotential for formic acid evolution. Our analysis also clarifies the importance of the reaction condition for CO2 reduction to liquid fuels utilizing RuO2-based electrocatalysts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Bhowmik, A. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 18333-18343
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 121
Issue number: 34
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
To study the role of novel Gd$_2$Zr$_2$O$_7$/Ce$_{0.9}$La$_{0.1}$O$_2$ buffer layer structure on a biaxially textured NiW substrate, a set of YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) films with different thickness were prepared by pulsed laser deposition (PLD). Interface imperfections as well as thickness-dependent structural properties were observed in the YBCO thin films. The structure is also reflected into the improved superconducting properties with the highest critical current densities in films with intermediate thicknesses. Therefore, it can be concluded that the existing buffer layers need more optimization before they can be successfully used for films with various thicknesses. This issue is linked to the extremely susceptible growth method of PLD when compared to the commonly used chemical deposition methods. Nevertheless, PLD-grown films can give a hint on what to concentrate to be able to further improve the buffer layer structures for future coated conductor technologies.

**General information**

State: Published

Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Turku

Authors: Malmivirta, M. (Ekstern), Huhtinen, H. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern), Paturi, P. (Ekstern)
Three-dimensional graphene anchored Fe\textsubscript{2}O\textsubscript{3}@C core-shell nanoparticles as supercapacitor electrodes

Three-dimensional (3D) reduced graphene oxide (rGO) anchored carbon-coated Fe\textsubscript{2}O\textsubscript{3} core-shell nanoparticles (Fe\textsubscript{2}O\textsubscript{3}@C-rGO) has been developed successfully through a simple one-pot hydrothermal process followed by a further annealing treatment. The 3D Fe\textsubscript{2}O\textsubscript{3}@C-rGO nanocomposite consists of carbon-coated Fe\textsubscript{2}O\textsubscript{3} nanoparticle clusters (Fe\textsubscript{2}O\textsubscript{3}@C) and rGO nanosheets. The homogenously distributed and intercalated Fe\textsubscript{2}O\textsubscript{3}@C nanoparticles between rGO nanosheets form a highly conductive 3D carbon network with rGO, and present a hierarchical pore size structure, enabling fast ion and electron transport, as well as remarkable specific surface area. The electrochemical performance in supercapacitor has been characterized, and the as-prepared Fe\textsubscript{2}O\textsubscript{3}@C-rGO electrode shows a significant high specific capacitance of 211.4 F/g at 0.5 A/g and 177.2 F/g at 20 A/g with no visible performance decay even after 2500 cycles testing. These properties indicate a good potential to achieve high performance electrochemical devices.
Topology optimization of heat exchangers and heat sinks

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Haertel, J. H. K. (Intern), Lei, T. (Intern), Alexandersen, J. (Intern), Engelbrecht, K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from Danish Days on Caloric Materials and Devices, Roskilde, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions: DanishDays2017_Abstract_Haertel.pdf
Publication: Research - peer-review > Conference abstract for conference – Annual report year: 2017

Topology optimized permanent magnet systems
Topology optimization of permanent magnet systems consisting of permanent magnets, high permeability iron and air is presented. An implementation of topology optimization for magnetostatics is discussed and three examples are considered. The Halbach cylinder is topology optimized with iron and an increase of 15% in magnetic efficiency is shown. A topology optimized structure to concentrate a homogeneous field is shown to increase the magnitude of the field by 111%. Finally, a permanent magnet with alternating high and low field regions is topology optimized and a $\Lambda_{cool}^\Lambda$ figure of merit of 0.472 is reached, which is an increase of 100% compared to a previous optimized design.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Bahl, C. (Intern), Insinga, A. R. (Intern)
Pages: 78-85
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Toward a drone-based EL and PL inspection tool for PV power plants

On-site inspection of PV systems has been historically performed through visual inspection, infrared (IR) thermography, and electrical measurements. Recent advances and cost reductions in unmanned aerial vehicle (UAV) technology have led to adoption of UAVs equipped with thermal cameras for inspection of PV plants, which survey power plants in a fraction of the time and cost than walk through IR imaging. IR imaging, however, is limited only to detection of certain fault types that result in elevated temperatures. Techniques such as electro-(EL) and photo-(PL) luminescence imaging offer a higher level of image detail and qualitative insight compared to IR thermography. Furthermore, detection and identification of incipient or severe faults in PV panels is more straightforward. This project proposes for the first time a fast and accurate automatic drone-based inspection method for large PV plants that combines IR, EL, PL imaging, and visual images (VI), called DronEL. The overarching goal is to correlate these images with known PV failures such as hotspots, cell cracks, and potential induced degradation. The DronEL project is carried out by a number of academic and commercial partners including Denmark’s Technical University (DTU), Aalborg University (AAU), Sky-watch, SiCon and Kenergy.

Towards a stable ion-solvating polymer electrolyte for advanced alkaline water electrolysis

Advanced alkaline water electrolysis using ion-solvating polymer membranes as electrolytes represents a new direction in the field of electrochemical hydrogen production. Polybenzimidazole membranes equilibrated in aqueous KOH combine the mechanical robustness and gas-tightness of a polymer with the conductive properties of an aqueous alkaline salt solution, and are thus of particular interest in this field of research. This work presents a comprehensive study of ternary alkaline polymer electrolyte systems developed around a polybenzimidazole derivative that is structurally tailored towards improved stability in alkaline environments. The novel electrolytes are extensively characterized with respect to physicochemical and electrochemical properties and the chemical stability is assessed in 0-50 wt% aqueous KOH for more than 6 months at 88 degrees C. In water electrolysis tests using porous 3-dimensional electrodes completely free from noble metals, they show polarization characteristics comparable to those of commercially available separators and good performance stability over several days.
Towards High Power Density Metal Supported Solid Oxide Fuel Cell for Mobile Applications

For use of metal supported SOFC in mobile applications it is important to reduce the thermal mass to enable fast start up, increase stack power density in terms of weight and volume and reduce costs. In the present study, we report on the effect of reducing the support layer thickness of 313 μm in DTU SoA MS-SOFCs gradually to 108 μm. The support layer thickness decrease in the DTU co-sintering MS-SOFC fabrication route results in an increased densification of the support layer and a slight decrease in performance. To mitigate the performance loss, the introduction of gas channels by puncturing of the green tape casted support layer was explored. In summary, it was successfully demonstrated on stack relevant sized 12 cm x 12 cm MS-SOFCs that the support layer thickness could be significantly reduced and that the cell performance could be significantly increased by the introduction of gas channels.
Towards identifying the active sites on RuO$_2$(110) in catalyzing oxygen evolution

While the surface atomic structure of RuO$_2$ has been well studied in ultra high vacuum, much less is known about the interaction between water and RuO$_2$ in aqueous solution. In this work, in situ surface X-ray scattering measurements combined with density functional theory (DFT) were used to determine the surface structural changes on single-crystal RuO$_2$(110) as a function of potential in acidic electrolyte. The redox peaks at 0.7, 1.1 and 1.4 V vs. reversible hydrogen electrode (RHE) could be attributed to surface transitions associated with the successive deprotonation of –H$_2$O on the coordinatively unsaturated Ru sites (CUS) and hydrogen adsorbed to the bridging oxygen sites. At potentials relevant to the oxygen evolution reaction (OER), an –OO species on the Ru CUS sites was detected, which was stabilized by a neighboring –OH group on the Ru CUS or bridge site. Combining potential-dependent surface structures with their energetics from DFT led to a new OER pathway, where the deprotonation of the –OH group used to stabilize –OO was found to be rate-limiting.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Theoretical Atomic-scale Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Massachusetts Institute of Technology, SLAC National Accelerator Laboratory, Argonne National Laboratory, Oregon State University, University of Copenhagen
Pages: 2626-2637
Towards long-term stable solid state electrolyzers with infiltrated catalysts

Renewable energy sources like wind and solar are widely considered as the key technologies to cover our growing demands. However, the fluctuating nature of these sources requires a flexible energy system and storage technologies to ensure that energy supply can be covered in a stable and affordable manner. One of the promising solutions is the production of synthetic fuel by solid oxide electrolyzers. Electricity can be converted to gas and further to liquid products during times of electricity production excess. In times of need, these fuels can be converted back to electricity by either conventional power plants or fuel cells.

Key challenges for a successful commercialization of solid oxide electrolyzers are upscale it, reduce cost and improve durability. Therefore, large efforts are allocated to improve cell performance. As a relatively novel method to introduce electro-catalysts into the porous structure of the electrodes, infiltration has shown very efficient. Solid oxide cells with infiltrated electrodes have been reported to show improved performance compared to conventional cells [1].

In this study, the development of infiltration procedures to improve the stability and catalytic performance of the fuel electrode of solid state electrolyzers (SOEC) will be presented. The infiltration process was optimized through choice of surfactants and concentrations of precursor solutions, to ensure easy penetration of the precursor solution into a Ni-YSZ (yttrium stabilized zirconia) composite backbone. The influence of surfactants on the coverage of specific grains with the infiltrated Ce0.8Gd0.2O2-d (CGO) nano-sized catalyst in the composite backbone was also studied. The optimized infiltration process was applied to 5 x 5 cm solid oxide cells.

The cells composed of a thin YSZ electrolyte, a Ni-YSZ fuel electrode and an LSCF-CGO oxygen electrode were tested in steam electrolysis operation under a current load of up to 1.25 A/cm². Under high steam content and high current density,
a fast cell degradation (~700 mV/kh) was observed for un-infiltrated cells. The infiltration of a CGO nano-sized catalyst into the Ni-YSZ backbone was observed to reduce the degradation rate to around 117 mV/kh.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Applied Electrochemistry, Imaging and Structural Analysis  
**Authors:** Ovtar, S. (Intern), Chen, M. (Intern), Brodersen, K. (Intern), Hauch, A. (Intern), Sun, X. (Intern), Bentzen, J. J. (Intern), Hendriksen, P. V. (Intern)  
**Number of pages:** 1  
**Publication date:** 2017  
**Event:** Abstract from 21st International Conference on Solid State Ionics, Padova, Italy.  
**Main Research Area:** Technical/natural sciences  
**Electronic versions:** SSI_infiltration_Ovtar.pdf  
**Source:** PublicationPreSubmission  
**Source-ID:** 134385065  
**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography**

Solid oxide cells (SOCs) offer great prospects for the efficient and reversible conversion of chemical to electrical energy. Therefore, they are expected to play a key role in the renewable energy landscape. However, their limited lifetime under operating conditions hinders their widespread usage. The degradation processes are mainly attributed to morphological changes occurring within the electrodes microstructure. Therefore, precise tracking of 3D microstructural evolution during operation is considered crucial to understanding the complex relationship between microstructure and performance.

In this work, X-ray ptychographic tomography is applied to SOC materials, demonstrating unprecedented spatial resolution and data quality. The eect of a complete redox cycle on the same Ni-YSZ microstructure is visualized ex-situ in 3D, showing major rearrangement of the nickel network after reduction, the formation of cracks in the YSZ, and void formation in nickel oxide after oxidation.

Capitalizing on the high resolution of ptychography, the eect of nickel coarsening on the Ni-YSZ microstructure evolution is studied ex-situ in three dimensions, while the sample is repeatedly scanned and treated at high temperature in dry hydrogen. The analyses show the substantial evolution of the nickel and pore networks during the rst 3 hours of treatment. The nickel coarsening leads to loss of nickel connectivity, a decrease in specific interface area and a decrease in total triple phase boundary density.

The ex-situ experiment on a redox cycle provides new insights on the nature of the redox processes occurring within a SOC fuel electrode. However, only the initial and nal steps of the reactions can be analyzed. To gain information about the intermediate steps of the reduction and oxidation, in-situ holographic tomography is applied. Preliminary results show rapid kinetics for the two reactions. During oxidation, void formation in metallic particles is observed. During reduction, the nickel oxide particles rst evolve to a nano-porous system of nickel crystallites and then coarsen towards dense nickel particles.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Imaging and Structural Analysis  
**Authors:** De Angelis, S. (Intern), Bowen, J. R. (Intern), Jørgensen, P. S. (Intern), Lauridsen, E. M. (Intern)  
**Number of pages:** 128  
**Publication date:** 2017

**Publication information**

**Publisher:** Department of Energy Conversion and Storage, Technical University of Denmark  
**Original language:** English  
**Main Research Area:** Technical/natural sciences  
**Electronic versions:** finalDef2.pdf

**Relations**

**Projects:**  
Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography  
**Source:** PublicationPreSubmission  
**Source-ID:** 139843599  
**Publication:** Research › Ph.D. thesis – Annual report year: 2017
Transient deformational properties of high temperature alloys used in solid oxide fuel cell stacks

Stresses and probability of failure during operation of solid oxide fuel cells (SOFCs) is affected by the deformational properties of the different components of the SOFC stack. Though the overall stress relaxes with time during steady state operation, large stresses would normally appear through transients in operation including temporary shut downs. These stresses are highly affected by the transient creep behavior of metallic components in the SOFC stack. This study investigates whether a variation of the so-called Chaboche's unified power law together with isotropic hardening can represent the transient behavior of Crofer 22 APU, a typical iron-chromium alloy used in SOFC stacks. The material parameters for the model are determined by measurements involving relaxation and constant strain rate experiments. The constitutive law is implemented into commercial finite element software using a user-defined material model. This is used to validate the developed constitutive law to experiments with constant strain rate, cyclic and creep experiments. The predictions from the developed model are found to agree well with experimental data. It is therefore concluded that Chaboche's unified power law can be applied to describe the high temperature inelastic deformational behaviors of Crofer 22 APU used for metallic interconnects in SOFC stacks.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Central Florida
Authors: Tadesse Molla, T. (Intern), Kwok, K. (Intern), Frandsen, H. L. (Intern)
Pages: 8-16
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 351
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
Transportable Device for Transference of Atmosphere Sensitive Materials from Glove Box to High Resolution Scanning Electron Microscope

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Wichmann, M. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at The 68th Annual Conference of the Nordic Microscopy Society (SCANDEM 2017), Reykjavík, Iceland.
Main Research Area: Technical/natural sciences
Electronic versions:
Scandem_2017_poster_jabe.pdf
Source: PublicationPreSubmission
Source-ID: 137101329
Publication: Research › Poster – Annual report year: 2017

Transportable Device for Transference of Atmosphere Sensitive Materials from Glove Box to High Resolution Scanning Electron Microscope

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Wichmann, M. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from The 68th Annual Conference of the Nordic Microscopy Society (SCANDEM 2017), Reykjavík, Iceland.
Main Research Area: Technical/natural sciences
Transfer device, Air sensitive materials, Glove box, HRSEM, High energy battery
Electronic versions:
Scandem2017_abstract_jabe_final.pdf
Source: PublicationPreSubmission
Source-ID: 137101307
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017
Transport and excitations in a negative-U quantum dot at the LaAlO₃/SrTiO₃ interface

In a solid-state host, attractive electron–electron interactions can lead to the formation of local electron pairs which play an important role in the understanding of prominent phenomena such as high Tc superconductivity and the pseudogap phase. Recently, evidence of a paired ground state without superconductivity was demonstrated at the level of single electrons in quantum dots at the interface of LaAlO₃ and SrTiO₃. Here, we present a detailed study of the excitation spectrum and transport processes of a gate-defined LaAlO₃/SrTiO₃ quantum dot exhibiting pairing at low temperatures. For weak tunneling, the spectrum agrees with calculations based on the Anderson model with a negative effective charging energy U, and exhibits an energy gap corresponding to the Zeeman energy of the magnetic pair-breaking field. In contrast, for strong coupling, low-bias conductance is enhanced with a characteristic dependence on temperature, magnetic field and chemical potential consistent with the charge Kondo effect.

General information

State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Copenhagen
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Nature Communications
Volume: 8
Issue number: 1
Article number: 395
ISSN (Print): 2041-1723
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.399 SNIP 2.995
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.364 SNIP 3.053 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.331 SNIP 3.091 CiteScore 10.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.967 SNIP 2.776 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.586 SNIP 2.724 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.122 SNIP 1.544 CiteScore 4.44
ISI indexed (2011): ISI indexed no
Web of Science (2010): Indexed yes

Original language: English
Electronic versions:
s41467_017_00495_7.pdf
DOIs:
10.1038/s41467-017-00495-7
Source: Findit
Source-ID: 2373350449
Publication: Research - peer-review » Journal article – Annual report year: 2017
Tuning the ground state of polar LaAlO$_3$/SrTiO$_3$ interface by an electron sink

Most of the intriguing properties of two-dimensional electron gases (2DEGs) at the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface are sensitive to the electrons located in 3d-orbit of Ti. However, tuning the electronic structure of the system remains challenging due to the intrinsic high carrier density. Herein, instead of using LaMnO$_3$ (LMO) as buffer layers [1], we show that Mn doping in LaAlO$_3$ (LAMO) creates an electron sink that alters the ground state of 2DEG by suppressing the carrier density at the interface, without changing the polarity of the system. By precise control of the Mn-doping level, we found that 2DEGs in our system experience a change from two-band to one-band transport with decreasing carrier density, which is accompanied by a Lifshitz transition at a critical carrier density of $2.76 \times 10^{13}$ cm$^{-2}$ at 2K. Significantly, the peak value (255.7 mK) of superconducting transition temperature is observed at Lifshitz point. In addition, our experiments realize the coexistence of ferromagnetism (FM) and superconductivity (SC) by Mn doping.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, University of Copenhagen
Number of pages: 1
Publication date: 2017
Event: Abstract from 24th International Workshop on Oxide Electronics (iWOE 2017), Chicago, Illinois, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Yulin_Gan.pdf
Source: PublicationPreSubmission
Source-ID: 140695841
Publication: Research › Conference abstract for conference – Annual report year: 2017

Tuning the Two-Dimensional Electron Gas at Oxide Interfaces with Ti-O Configurations: Evidence from X-ray Photoelectron Spectroscopy

Chemical redox reaction can lead to a two-dimensional electron gas (2DEG) at the interface between a TiO$_2$-terminated SrTiO$_3$ (STO) substrate and an amorphous LaAlO$_3$ (a-LAO) capping layer. When replacing the STO substrate with rutile and anatase TiO$_2$ substrates, considerable differences in interfacial conduction are observed. Based on X-ray photoelectron spectroscopy (XPS) and transport measurements, we conclude that the interfacial conduction comes from redox reactions, and that the differences among the materials systems result mainly from variations in the activation energies for the diffusion of oxygen vacancies at substrate surfaces.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences, Technical University of Denmark
Number of pages: 26
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Tuning the two-dimensional electron liquid at oxide interfaces by buffer-layer-engineered redox reactions

Polar discontinuities and redox reactions provide alternative paths to create two-dimensional electron liquids (2DELs) at oxide interfaces. Herein, we report high mobility 2DELs at interfaces involving SrTiO$_3$ (STO) achieved using polar La$_{7/8}$Sr$_{1/8}$MnO$_3$ (LSMO) buffer layers to manipulate both polarities and redox reactions from disordered overlayers grown at room temperature. Using resonant x-ray reflectometry experiments, we quantify redox reactions from oxide overlayers on STO as well as polarity induced electronic reconstruction at epitaxial LSMO/STO interfaces. The analysis reveals how these effects can be combined in a STO/LSMO/disordered film trilayer system to yield high mobility modulation doped 2DELs, where the buffer layer undergoes a partial transformation from perovskite to brownmillerite structure. This uncovered interplay between polar discontinuities and redox reactions via buffer layers provides a new approach for the design of functional oxide interfaces.
Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Technical University of Denmark
Number of pages: 1
Publication date: 2017
Event: Abstract from 3rd Functional Oxide Thin Films for Advanced Energy and Information Technology Conference, Rome, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:
abstract_Yunzhong_Modulation_doped_2DEG.pdf
Source: PublicationPreSubmission
Source-ID: 140346906
Publication: Research › Conference abstract for conference – Annual report year: 2017

Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Ultrasensitive binder-free glucose sensors based on the pyrolysis of in situ grown Cu MOF

A non-enzymatic glucose sensor based on carbon/Cu composite materials was developed by the in-situ growth and subsequent pyrolysis of metal-organic frameworks (MOFs) on Cu foam. After pyrolysis, SEM, HRTEM and STEM-EELS were employed to clarify the hierarchical Cu@porous carbon electrode. It is found that the Cu nanoparticles are uniformly embedded in the carbon matrix, attached on the carbon layer closely. The electrocatalytic activity of the Cu@porous carbon matrix electrode for glucose sensing was explored by cyclic voltammetry (CV) and chronamperometry. The resulting Cu@porous carbon matrix electrode displays ultrahigh sensitivity (10.1 mA cm⁻² mM⁻¹), low detection limit (<1 μM), short response time (less than 2 s) and good stability, indicating that the developed electrode is a promising candidate material for glucose sensors.
Ultra-thin Cu2ZnSnS4 solar cell by pulsed laser deposition

We report on the fabrication of a 5.2% efficiency Cu2ZnSnS4 (CZTS) solar cell made by pulsed laser deposition (PLD) featuring an ultra-thin absorber layer (less than 450 nm). Solutions to the issues of reproducibility and micro-particulate ejection often encountered with PLD are proposed. At the optimal laser fluence, amorphous CZTS precursors with optimal stoichiometry for solar cells are deposited from a single target. Such precursors do not result in detectable segregation of secondary phases after the subsequent annealing step. In the analysis of the solar cell device, we focus on the effects of the finite thickness of the absorber layer. Depletion region width, carrier diffusion length, and optical losses due to incomplete light absorption and back contact reflection are quantified. We conclude that material- and junction quality is comparable to that of thicker state-of-the-art CZTS devices, even though the efficiency is lower due to optical losses.

General information

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials, The VILLUM Center for the Science for Sustainable Fuels and Chemicals, University of New South Wales, Technical University of Denmark
Authors: Cazzaniga, A. C. (Intern), Crovetto, A. (Intern), Yan, C. (Ekstern), Sun, K. (Ekstern), Hao, X. (Ekstern), Estelrich, J. R. (Ekstern), Canulescu, S. (Intern), Stamate, E. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern)
Pages: 91–99
Publication date: 2017
Main Research Area: Technical/natural sciences
Understanding the Capacitance of PEDOT:PSS

Poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) is the most studied and explored mixed ion-electron conducting polymer system. PEDOT:PSS is commonly included as an electroactive conductor in various organic devices, e.g., supercapacitors, displays, transistors, and energy-converters. In spite of its long-term use as a material for storage and transport of charges, the fundamentals of its bulk capacitance remain poorly understood. Generally, charge storage in supercapacitors is due to formation of electrical double layers or redox reactions, and it is widely accepted that PEDOT:PSS belongs to the latter category. Herein, experimental evidence and theoretical modeling results are reported that significantly depart from this commonly accepted picture. By applying a two-phase, 2D modeling approach it is demonstrated that the major contribution to the capacitance of the two-phase PEDOT:PSS originates from electrical double layers formed along the interfaces between nanoscaled PEDOT-rich and PSS-rich interconnected grains that comprises two phases of the bulk of PEDOT:PSS. This new insight paves a way for designing materials and devices, based on mixed ion-electron conductors, with improved performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linköping University
Number of pages: 10
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 27
Issue number: 28
Article number: 1700329
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Unique Crystal Orientation of Poly(ethylene oxide) Thin Films by Crystallization Using a Thermal Gradient

Poly(ethylene oxide), (PEO), thin films of different thicknesses (220, 450, and 1500 nm) and molecular masses (4000, 8000, and 20000 g/mol) have been fabricated by spin-coating of methanol solutions onto glass substrates. All these samples have been recrystallized from the melt using a directional thermal gradient technique. Millimeter-size domains with crystallites uniformly, oriented in the direction of the thermal gradient are observed. Furthermore, the crystallites size and orientation distribution are enhanced (e.g., increases and decreases, respectively) when film thickness is decreased, ultimately leading to a single-crystal-like behavior for 220 nm thick PEO films of mass 8000 g/mol. Interestingly, this fine microstructure is; partially retained after melting and subsequent-cooling back to ambient temperature for the highest molecular weight polymer allowing, in this particular case, to significantly decrease the distribution of crystal orientation obtained after crystallization using the thermal gradient technique.
Universality of electron mobility in LaAlO$_3$/SrTiO$_3$ and bulk SrTiO$_3$

Metallic LaAlO$_3$/SrTiO$_3$ (LAO/STO) interfaces attract enormous attention, but the relationship between the electron mobility and the sheet electron density, $n_{\text{3D}}$, is poorly understood. Here, we derive a simple expression for the three-dimensional electron density near the interface, $n_{\text{3D}}$, as a function of $n_{\text{s}}$, and find that the mobility for LAO/STO-based interfaces depends on $n_{\text{3D}}$ in the same way as it does for bulk doped STO. It is known that undoped bulk STO is strongly compensated with $N$ similar or equal to $5 \times 10^{18}$ cm$^{-3}$ background donors and acceptors. In intentionally doped bulk STO with a concentration of electrons $n_{\text{3D}} < N$, background impurities determine the electron scattering. Thus, when $n_{\text{3D}} < N$, it is natural to see in LAO/STO the same mobility as in the bulk. On the other hand, in the bulk samples with $n_{\text{3D}} > N$, the mobility collapses because scattering happens on $n_{\text{3D}}$ intentionally introduced donors. For LAO/STO, the polar catastrophe which provides electrons is not supposed to provide an equal number of random donors and thus the mobility should be larger. The fact that the mobility is still the same implies that for the LAO/STO, the polar catastrophe model should be revisited.
Unlocking the Electrocatalytic Activity of Chemically Inert Amorphous Carbon-Nitrogen for Oxygen Reduction: Discerning and Refactoring Chaotic Bonds

Mild annealing enables inactive nitrogen (N)-doped amorphous carbon (a-C) films abundant with chaotic bonds prepared by magnetron sputtering to become effective for the oxygen reduction reaction (ORR) by virtue of generating pyridinic N. The rhythmic variation of ORR activity elaborates well on the subtle evolution of the amorphous C−N bonds conferred by spectroscopic analysis.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Jilin University
Using ISOS consensus test protocols for development of quantitative life test models in ageing of organic solar cells

As Organic Photovoltaic (OPV) development matures, the demand grows for rapid characterisation of degradation and application of Quantitative Accelerated Life Tests (QALT) models to predict and improve reliability. To date, most accelerated testing on OPVs has been conducted using ISOS consensus standards. This paper identifies some of the problems in using and interpreting the results for predicting ageing based upon ISOS consensus standard test data. Design of Experiments (DOE) in conjunction with data from ISOS consensus standards are used as the basis for developing life test models for OPV modules. This is used to study their temperature-humidity and light-induced degradation, which enables failure rates during accelerated testing to be assessed against the typical outdoor operational conditions. The life test models are used to assess the relative severity of the ISOS standards and the impact of geographic and seasonal climatic changes on OPV degradation.
Voltage and Thermally Driven Roll-to-Roll Organic Printed Transistor Made in Ambient Air Conditions

Resume: Organic thin film transistors offer great potential for use in flexible electronics. Much of this potential lies in the solution processability of the organic polymers enabling both roll coating and printing on flexible substrates and thus greatly reducing the material and fabrication costs. We present flexible organic power transistors prepared by fast (20 m min$^{-1}$) roll-to-roll flexographic printing of the drain and source electrode structures, with an interspace below 50 um, directly on polyester foil[1]. The devices have top gate architecture and were completed by slotdie coating of the organic
semiconductor poly3hexylthiophene and the dielectric material polyvinylphenol before the gate was applied by screen printing. All the processing was realized in ambient air on a PET flexible substrate. We explore the footprint and the practically accessible geometry of such devices with a special view toward being able to drive large currents while handling the thermal aspects in operation together with other organic printed electronics technologies such as large area organic photovoltaics (OPV) and large area electrochromic displays (EC). We find especially that an elevated operational temperature is beneficial with respect to both transconductance and on/off ratio. We achieve high currents of up to 45 mA at a temperature of 80 °C. Finally, we observe a significant temperature dependence of the performance, which can be explored further in sensing applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Links:

Bibliographical note
Source: PublicationPreSubmission
Source-ID: 134441457
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Waste to energy plant operation under the influence of market and legislation conditioned changes
In this paper, gate-fee changes of the waste-to-energy plants are investigated in the conditions set by European Union legislation and by the introduction of the new heat market. Waste management and sustainable energy supply are core issues of sustainable development of regions, especially urban areas. These two energy flows logically come together in the combined heat and power facility by waste incineration. However, the implementation of new legislation influences quantity and quality of municipal waste and operation of waste-to-energy systems. Once the legislation requirements are met, waste-to-energy plants need to be adapted to market operation. This influence is tracked by the gate-fee volatility. The operation of the waste-to-energy plant on electricity markets is simulated by using EnergyPLAN and heat market is simulated in Matlab, based on hourly marginal costs. The results have shown that the fuel switch reduced gate-fee and made the facility economically viable again. In the second case, the operation of the waste-to-energy plant on day-ahead electricity and heat market is analysed. It is shown that introducing heat market increased needed gate-fee on the yearly level over the expected levels. Therefore, it can be concluded that the proposed approach can make projects of otherwise questionable feasibility more attractive.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, University of Zagreb, SDEWES Centre
Authors: Tomic, T. (Ekstern), Dominkovic, D. F. (Intern), Pfeifer, A. (Ekstern), v, D. R. (Ekstern), Pedersen, A. S. (Intern), Duić, N. (Ekstern)
Pages: 1119-1129
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy
Volume: 137
ISSN (Print): 0360-5442
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.17 SJR 1.999 SNIP 1.798
Web of Science (2016): Indexed yes
When two become one: an insight into 2D conductive oxide interfaces

Recent progress has led to conductance confinement at the interface of complex oxide heterostructures, thereby providing new opportunities to explore nano-electronic as well as nano-ionic devices. In this paper we describe how interfacial contiguity between materials can trigger redox reactions inducing metallic conductivity along the interface of SrTiO₃-based heterostructures and create new types of 2 Dimension Electron Gases (2DEG) at the hetero-interface with electron mobility enhancements of more than one order of magnitude higher than those of hitherto investigated perovskite-type interfaces. Furthermore, our recent results, examining strain effects at interfaces, demonstrate the potential of achieving hetero-epitaxial thin films with superior ionic or electronic properties. We also present a novel concept that uncovers a wide variety of possible technological opportunities for materials design utilizing ionic conducting multi-layered...
heterostructures. These findings hold the potential to pave the way for novel and/or superior all-oxide electronic and ionic devices.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science
Authors: Pryds, N. (Intern), Esposito, V. (Intern)
Pages: 1-23
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Electroceramics
Volume: 38
Issue number: 1
ISSN (Print): 1385-3449
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.15 SJR 0.429 SNIP 0.561
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.568 SNIP 0.761 CiteScore 1.49
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.598 SNIP 0.831 CiteScore 1.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.555 SNIP 1.101 CiteScore 1.43
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.642 SNIP 1.092 CiteScore 1.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.482 SNIP 0.768 CiteScore 1.07
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.627 SNIP 0.837
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.695 SNIP 0.769
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.682 SNIP 0.775
Scopus rating (2007): SJR 0.579 SNIP 0.584
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.857 SNIP 1.158
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.744 SNIP 0.928
Scopus rating (2004): SJR 0.909 SNIP 1.332
Scopus rating (2003): SJR 0.755 SNIP 0.929
Scopus rating (2002): SJR 0.571 SNIP 0.825
Scopus rating (2001): SJR 0.579 SNIP 0.644
Scopus rating (2000): SJR 0.793 SNIP 0.796
X-Ray and Raman studies on all-solid-state Li-S batteries built around LiBH4 solid electrolyte

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Das, S. (Intern), Blanchard, D. (Intern)
Number of pages: 2
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
X-Ray_and_Raman_studies_on_all_solid_state_Li_S_batteries_built_around_LiBH4_solid_electrolyte.pdf
Links:
http://www.lism3.org/
Source: PublicationPreSubmission
Source-ID: 130762767
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

X-Ray microtomography studies on all-solid-state Li-S batteries built around LiBH4 solid electrolyte

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017
Host publication Information
Title of host publication: Proceedings of the Danscatt Annual meeting 2017
Main Research Area: Technical/natural sciences
Conference: Danscatt Annual meeting 2017, Odense, Denmark, 01/06/2017 - 01/06/2017
Links:
Source: PublicationPreSubmission
Source-ID: 132365165
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Zirconia nano-colloids transfer from continuous hydrothermal synthesis to inkjet printing
Water dispersions of nanometric yttria stabilized zirconia (YSZ) particles synthesized by Continuous Hydrothermal Synthesis are transferred into nano-inks for thin film deposition. YSZ nanoparticles are synthesized in supercritical conditions resulting in highly dispersed crystals of 10 nm in size. The rheology of the colloid is tailored to achieve inkjet printability (Z) by using additives for regulating viscosity and surface tension. Inks with a wide range of properties are produced. A remarkable effect of nanoparticles on the ink printability is registered even at solid load < 1%vol. In particular, nanoparticles hinder the droplet formation at low values of the printability while suitable jetting is observed at high Z values, i.e. Z = 20. For the optimized inks, we achieve high quality printing with lateral and thickness resolutions of 70 μm and ca. 250 nm respectively, as well as self-levelling effect with a reduction of the substrate roughness. Densification is achieved at sintering temperatures below 1200 °C.
Partially fluorinated electrospun proton exchange membranes

The present invention relates to a novel porous membrane layer, to a novel method for producing a membrane, and the membranes produced by the novel method. The present invention further relates to a fuel cell comprising the porous layer, as well as any use of the porous layer in a fuel cell or in a filter. The porous membrane layer comprises a plurality of randomly oriented fibers manufactured by electrospinning, wherein the fibers comprise a graft copolymer, wherein the graft copolymer comprises a backbone and at least one side chain, wherein the backbone comprises a partially fluorinated copolymer, and wherein at least one side chain of the graft copolymer comprises a polymerization product of a polymerizable proton donor group or a precursor thereof.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Energy Conversion and Storage
Authors: Javakhishvili, I. (Intern), Hvilsted, S. (Intern), Jankova Atanasova, K. (Intern)
Publication date: 24 Nov 2016

Publication information
IPC: H01M 8/ 10 A I
Patent number: WO2016185009
Date: 24/11/2016
Priority date: 20/05/2015
Priority number: EP20150168423
Original language: English
Electronic versions:
WO2016185009A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016185009
Publication: Research › Patent – Annual report year: 2016

Gas sensor with multiple internal reference electrodes and sensing electrodes

The invention relates to a potentiometric gas sensor, or potentiometric gas detection element, with multiple internal reference electrodes and multiple sensing electrodes for determining the concentrations of gas components in a gaseous mixture. The sensor for gas detection comprises: a solid electrolyte, at least two sensing electrodes (SEs) in solid contact with the electrolyte, and at least two internal reference electrodes (IREs) in solid contact with the electrolyte, wherein each IRE comprises a composite material, comprising a binary mixture of a metal and a metal oxide dispersed to form a three-dimensional network extending throughout the IRE, and wherein each SE is electrically connected with at least one IRE.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Hu, Q. (Intern), Mogensen, M. B. (Intern)
Publication date: 20 Oct 2016

Publication information
IPC: G01N 33/ 00 A I
Patent number: WO2016166126
Date: 20/10/2016
Priority date: 13/04/2015
Priority number: EP20150163339
Dual-role plasticizer and dispersant for ceramic layers

Thus, one aspect of the invention relates to a green ceramic layer comprising a ceramic material, a binder, and a dual-role dispersant and plasticizer, wherein said dual-role dispersant and plasticizer is an organic di- or tri-ester selected from compounds of formula (I), (II), (III) and (IV). Another aspect of the present invention relates to a slurry for use in the manufacturing of a green ceramic layer comprising a ceramic material, a solvent, a binder, and a dual-role dispersant and plasticizer, wherein said dual role dispersant and plasticizer is an organic di- or tri-ester. Further aspects include uses of and methods of manufacturing said green ceramic layers.

Thermoelectric material comprising scandium doped zinc cadmium oxide

There is presented a composition of scandium doped Zinc Cadmium Oxide with the general formula ZnzCdxScyO which the inventors have prepared, and for which material the inventors have made the insight that it is particularly advantageous as an n-type oxide material, such as particularly advantageous for high temperature thermoelectric application with good TE properties and superior stability in air. In a particular embodiment, there is presented a material with the general formula Zn1-x-yCdxScyO, where 0.05
Polymer solution, fiber mat, and nanofiber membrane-electrode-assembly therewith, and method of fabricating same

In one aspect of the present invention, a fiber mat is provided. The fiber mat includes at least one type of fibers, which includes one or more polymers. The fiber mat may be a single fiber mat which includes one type of fibers, or may be a dual or multi fiber mat which includes multiple types of fibers. The fibers may further include particles of a catalyst. The fiber mat may be used to form an electrode or a membrane. In a further aspect, a fuel cell membrane-electrode-assembly has an anode electrode, a cathode electrode, and a membrane disposed between the anode electrode and the cathode electrode. Each of the anode electrode, the cathode electrode and the membrane may be formed with a fiber mat.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Pintauro, Peter, N. (Ekstern), Zhang, W. (. (Intern), Brodt, M. W. (Ekstern), Park, Andrew, M. (Ekstern), Ballenee, Jason, B. (Ekstern), Wycisk, R. (Ekstern)
Publication date: 31 Mar 2016

Publication information
IPC: H01M 8/10 A1
Patent number: WO2016048309
Date: 31/03/2016
Priority date: 24/09/2014
Priority number: WO2014US57278
Original language: English
Electronic versions:
WO2016048309A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016048309
Publication: Research › Patent – Annual report year: 2016

2D vs. 1D Structures at Stepped Si Surfaces and in Organic Molecules

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Wisconsin-Madison, Lawrence Berkeley National Laboratory, Naval Research Laboratory, University of Rostock, Universidad del Pais Vasco
Authors: Himpsel, F. (Ekstern), García Lastra, J. M. (Intern), Rubio, Á. (Ekstern), Boukahil, I. (Ekstern), Qiao, R. (Ekstern), Erwin, S. (Ekstern), Barke, I. (Ekstern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Pacific Rim Symposium on Surfaces, Coatings and Interfaces, Kohala Coast, HI, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
2D_vs_1D.pdf
Source: PublicationPreSubmission
Source-ID: 128083371
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

3D Mapping Of Density And Crack Propagation Through Sintering Of Catalysis Tablets By X-Ray Tomography
For hydrogen production, by steam reforming, porous ceramics are broadly used as catalyst support, due to their stability and ease in shaping. Catalyst supports in the form of tablets are conventionally produced by powder pressing and subsequent sintering. However, if the process is not done properly, cracks may arise and propagate during the sintering of the tablets. This can lead to weak sintered tablets that get rejected in the quality control. For this work, crack-containing samples of rejected tabletized support were provided. The formation, growth and closure of internal cracks during sintering of the rejected tabletized support material are studied by 3D X-ray tomography. This is a powerful technique, which due to its nondestructive nature is suitable to study the development of internal cracks in the tablets during sintering. Cracks could be identified in the green tablet (before sintering), which may indicate an uneven compaction of the powder, leading to an uneven spring-back after compaction. During sintering, some of the initial cracks were observed to close, while others were observed to open. Furthermore new cracks were also observed to arise during sintering. The different cracks locations and developments were analyzed in relationship to the surrounding microstructural features in an attempt to
A Cascading Model Of An Active Magnetic Regenerator System

In recent years, significant amounts of studies have been done on modeling and analysis of active magnetic regenerators (AMRs). Depending on the AMR geometry and the magnetocaloric material being modeled, the AMR may not be able to provide the required performance demanded by practical applications. Some AMR models in the literature predict high performance but with relatively low temperature spans at either end of the AMR. Therefore, they may not be sufficient for practical applications, such as providing the heat exchanger temperature spans required for residential and commercial space air conditioning. To remedy this, one solution is cascading of multiple single layer AMRs. In this work, a cascading AMR model is presented and studied. In a cascade configuration, N number of single layer AMRs are connected. The results show that higher hot and cold side temperature differences may be achieved compared to the ones obtained with a single AMR rendering the solution more suitable for use in residential and commercial space conditioning.

Accelerated ceria–zirconia solubilization by cationic diffusion inversion at low oxygen activity

Fast elemental diffusion at the Gd-doped ceria/Y-stabilized zirconia interface occurs under reducing conditions at low oxygen activity (pO2 < 10−12 atm) and high temperature (1400 °C). This effect leads to formation of thick ceria–zirconia solid solution reaction layers in the micro-range vs. thin layers of few tens of nanometers under oxidative conditions (i.e. in synthetic air at pO2 = 0.21 atm). The fast dissolution occurs by an inversion of the dominating limiting mechanism from the expected Zr4+ diffusion into the CGO lattice at high pO2 to an unexpected Ce3+ diffusion into the YSZ component under reducing conditions. The diffusion coefficient of 8-fold coordinated Ce3+ in YSZ at 1400 °C and pO2 = 10−13 atm is estimated to be around 10−11 cm2 s−1. This value is around 3 orders of magnitude higher than Zr4+ interdiffusion in CGO under oxidative conditions and about 8 orders of magnitude higher than Ce4+ self-diffusion in CGO in air at the same temperature.
Accelerated creep in solid oxide fuel cell anode supports during reduction

To evaluate the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. The creep of reduced Ni-YSZ anode support at operating conditions has been studied previously. In this work a newly discovered creep phenomenon taking place during the reduction is reported. This relaxes stresses at a much higher rate (∼ ×10^4) than creep during operation. The phenomenon was studied both in three-point bending and uniaxial tension. Differences between the two measurements could be explained by newly observed stress promoted reduction. Finally, samples exposed to a small tensile stress (∼ 0.004 MPa) were observed to expand during reduction, which is in contradiction to previous literature. These observations suggest that release of internal residual stresses between the NiO and the YSZ phases occurs during reduction. The accelerated creep should practically eliminate any residual stress in the anode support in an SOFC stack, as has previously been indirectly observed. This phenomenon has to be taken into account both in the production of stacks and in the simulation of the stress field in a stack based on anode supported SOFCs. (C) 2016 Elsevier B.V. All rights reserved.
Acid–Base Chemistry and Proton Conductivity

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Case Western Reserve University
Authors: Li, Q. (Intern), Aili, D. (Intern), Savinell, R. F. (Ekstern), Jensen, J. O. (Intern)
Pages: 37-57
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 3
Main Research Area: Technical/natural sciences
DOIs:
10.1007/978-3-319-17082-4_3
Publication: Research - peer-review › Book chapter – Annual report year: 2016

A contribution to the understanding of the combined effect of nitrogen and boron in grey cast iron

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Mixed Conductors, Dansk Udviklings Formidling ApS
Authors: Strande, K. (Ekstern), Tiedje, N. S. (Intern), Chen, M. (Intern)
Pages: 127-128
Publication date: 2016

Host publication information
Title of host publication: 72nd World Foundry Congress (WFC 2016): Proceedings of a meeting held 21-25 May 2016, Nagoya, Japan.
Publisher: World Foundry Organization
ISBN (Print): 9781510833128
Main Research Area: Technical/natural sciences
Conference: 72nd World Foundry Congress (WFC 2016), Nagoya, Japan, 21/05/2016 - 21/05/2016
Source: FindIt
Source-ID: 2393757283
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Active cooling of a down hole well tractor
Wireline interventions in high temperature wells represent one of today's biggest challenges for the oil and gas industry. The high wellbore temperatures, which can reach 200 °C, drastically reduce the life of the electronic components contained in the wireline downhole tools, which can cause the intervention to fail. Active cooling systems represent a possible solution to the electronics overheating, as they could maintain the sensitive electronics at a tolerable temperature, while operating in hotter environments. This work presents the design, construction and testing of an actively cooled
downhole electronics section, which is able to cool the critical electronics below 175 °C while operating at 200 °C. After the investigation of several cooling techniques and the thermal characterization of the studied downhole electronics, thermoelectric coolers were chosen to implement a novel concept of heat management for downhole tools. The chosen design combined active and passive cooling techniques aiming at efficient thermal management, preserving the tool compactness, and avoiding the use of moving parts. Topology optimization was used, in combination with a finite element model of the system, to develop the final design of an actively cooled prototype, which was able to continuously maintain the temperature-sensitive electronics below 170 °C, while operating at 200 °C for more than 200 hours. Effective electrical integration of the cooling system in a wireline downhole tool was also studied, and a power-width-modulation circuit was developed to adapt the downhole power source to a suitable voltage for the thermoelectric cooler. The implementation of the active cooling system was supported by the study of the thermal interaction between the downhole tool and the well environment, which was relevant to define the heat rejection conditions. Given the lack of information from the scientific literature, a downhole sensor that could experimentally quantify the heat transfer rate occurring between the tool and the wellbore was designed and tested. The concept was proved and the sensor calibrated in a laboratory flow loop. Average and maximum mismatches of 3% and 10%, respectively, were found between the measured and predicted heat transfer coefficients, showing good agreement between experimental results and model forecasts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Soprani, S. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Nesgaard, C. (Ekstern)
Number of pages: 253
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: Stefano_Soprani_PhD_Thesis_2016.pdf

Relations
Projects:
Active cooling of a down hole well tractor
Publication: Research › Ph.D. thesis – Annual report year: 2016

Active magnetic regenerator refrigeration with rotary multi-bed technology
Magnetic refrigeration is an emerging cooling technology with potential advantages over conventional vapor compression, the most important being higher efficiency. This thesis presents experimental and theoretical research into the possibilities of realizing this potential with actual active magnetic regenerator (AMR) prototypes. The starting point is the design and experiments with a rotary multi-bed prototype at the Technical University of Denmark. Promising results were obtained with this machine in terms of temperature span and cooling power. However, issues limiting the energy efficiency, mainly relating to heat leaks and flow system friction losses, have given rise to new ideas for taking the technology a step further. On this background, a second generation multi-bed prototype was designed, built and used in experimental investigations. A central feature of the new prototype is a novel system for handling the heat transfer fluid, providing a reciprocating flow inside the AMR beds while ensuring a continuous unidirectional flow in the surrounding flow circuit, communicating with the hot and cold reservoirs. With this system it is possible, via an arrangement of poppet valves and check valves, to control the flow rate versus rotational angle of the magnet system providing a time varying magnetic field in the beds with very minor losses compared to more traditional rotary valve based systems. Numerical AMR modeling capturing the variations in the azimuthal direction inside the beds has been used to investigate the effect of the shape of this flow profile, which confirms the importance of carefully optimizing it for the desired operating conditions. Numerical modeling and heat transfer calculations addressing heat leaks through the walls of the regenerator housing has revealed a necessary trade off between the amount of magnetocaloric material and an insulating air gap in the magnetized volume provided by the Halbach-like cylindrical permanent magnet system, when designing for high efficiency rather than maximum cooling power. The central part of the magnet system is a flux conducting iron core which was laminated for electrical and thermal insulation to minimize heat leaks and eddy current losses. Experimental investigations with different configurations of iron and insulation in the core focusing on the impact on temperature span and COP were conducted. AMR experiments with the new prototype revealed strong impacts on COP and cooling power by minor adjustments of the individual valves controlling the flow in each bed. This effect, inherent to rotary multibed AMRs, is ad- dressed with a numerical modeling approach and confirmed experimentally with the new prototype by carefully evening out the variations by the means of needle valves. An experimental performance analysis of the new prototype was carried out. A breakdown of the losses indicate pressure drop in external components and regenerator losses as the main contributors to entropy generation. While the former may be reduced by simple design improvements, the latter is non-trivial and requires detailed geometrical optimization assisted by numerical modeling and improved manufacturing techniques. Finally, possible applications are discussed and a concept of operating the AMR machine in combination with a thermal storage is introduced and demonstrated experimentally. Furthermore, a novel shunt valve technology, which was developed as a spin-off from the magnetic refrigeration research, is presented.
A Decade of Improvements for Solid Oxide Electrolysis Cells. Long-Term Degradation Rate from 40%/Knh to 0.4 % Knh

Solid oxide electrolysis cells (SOEC) have the potential for efficient large-scale conversion from electrical energy to chemical energy stored in fuels, such as hydrogen or synthetic hydrocarbon fuels by use of well-known catalysis processes. Key issues for the break-through of this technology are to provide inexpensive, reliable, high performing and long-term stable SOEC for stack and system applications. At DTU Energy (formerly Department of Fuel Cells and Solid State Chemistry, Risø National Laboratory), research within SOEC for more than a decade has led to long-term degradation rates on cell level being improved from 40 %/kh to 0.4 %/kh for tests at -1 A/cm² (figure 1). In this paper, we review the key findings and highlight different performance and durability limiting factors that have been discovered, analyzed and addressed over the years to reach the tremendous increase in long-term stability for SOEC as illustrated by the cell tests in figure 1.

A Density Functional Theory Study of the Ionic and Electronic Transport Mechanisms in LiFeBO₃ Battery Electrodes

Lithium iron borate is an attractive cathode material for Li-ion batteries due to its high specific capacity and low-cost, earth-abundant constituents. However, experiments have observed poor electrochemical performance due to the formation of an intermediate phase, that is, LiₓFeBO₃, which leads to large overvoltages at the beginning of charge. Using a convex-hull analysis, based on Hubbard-corrected density functional theory (DFT+U), we identify this intermediate phase as Li_{0.5}FeBO₃. Moreover, we show by means of the nudged elastic band (NEB) method, that the origin of these adverse electrochemical effects can be explained by an intrinsically low Li-ion and electron/hole-polaron mobility in Li_{0.5}FeBO₃ due to high activation barriers for both the ionic and electronic transport. These studies include the effects of the experimentally reported commensurate modulation. We have also investigated the Li-ion/hole diffusion through the interface between Li_{0.5}FeBO₃ and LiFeBO₃, which is found not to result in additional kinetic limitations from Li diffusion across the intraparticle interfaces. These findings suggest that the experimentally observed diminished performance associated with the formation of intermediate phases is linked to the intrinsically poor properties of the Li_{0.5}FeBO₃ phase rather than to the presence of interfaces between different phases.
A design approach for integrating thermoelectric devices using topology optimization

Efficient operation of thermoelectric devices strongly relies on the thermal integration into the energy conversion system in which they operate. Effective thermal integration reduces the temperature differences between the thermoelectric module and its thermal reservoirs, allowing the system to operate more efficiently. This work proposes and experimentally demonstrates a topology optimization approach as a design tool for efficient integration of thermoelectric modules into systems with specific design constraints. The approach allows thermal layout optimization of thermoelectric systems for different operating conditions and objective functions, such as temperature span, efficiency, and power recovery rate. As a specific application, the integration of a thermoelectric cooler into the electronics section of a downhole oil well intervention tool is investigated, with the objective of minimizing the temperature of the cooled electronics. Several challenges are addressed: ensuring effective heat transfer from the load, minimizing the thermal resistances within the integrated system, maximizing the thermal protection of the cooled zone, and enhancing the conduction of the rejected heat to the oil well. The design method incorporates temperature dependent properties of the thermoelectric device and other materials. The 3D topology optimization model developed in this work was used to design a thermoelectric system, complete with insulation and heat sink, that was produced and tested. Good agreement between experimental results and model forecasts was obtained and the system was able to maintain the load at more than 33 K below the oil well temperature. Results of this study support topology optimization as a powerful design tool for thermal design of thermoelectric systems.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Soprani, S. (Intern), Haertel, J. H. K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern), Engelbrecht, K. (Intern)
Pages: 49–64
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 176
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
A detailed study of the hysteresis in $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$

We report a thorough study of the thermal hysteresis behaviour of a single phase sample of the magnetocaloric material $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$. Previous reports in the literature have variously found hysteresis and non-hysteresis behaviour. We show the importance of measuring under carefully defined heating and cooling procedures. Careful analysis of the specific heat, measured at five different temperature ramp rates, and the magnetic entropy change indicates that there is no observable hysteresis, even though the behaviour of both quantities is consistent with a first-order phase transition. We discuss the reasons for this and for the differing results previously found.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. R. H. (Intern)
Pages: 429-433
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 416
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Scopus rating (2017): CiteScore 2.41 SJR 0.71 SNIP 1.22

BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
Web of Science (2013): Indexed yes

BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302 CiteScore 1.95
Web of Science (2012): Indexed yes

BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285 CiteScore 1.84
Web of Science (2011): Indexed yes

BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
Web of Science (2010): Indexed yes

BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
Web of Science (2009): Indexed yes

BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.861 SNIP 0.897
Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 0.708 SNIP 0.848
Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 0.832 SNIP 0.877
Web of Science (2006): Indexed yes

Scopus rating (2005): SJR 0.683 SNIP 0.693
Web of Science (2005): Indexed yes

Scopus rating (2004): SJR 0.792 SNIP 1.037
Web of Science (2004): Indexed yes

Scopus rating (2003): SJR 0.975 SNIP 0.897
Web of Science (2003): Indexed yes

Scopus rating (2002): SJR 1.188 SNIP 1.079
Web of Science (2002): Indexed yes

Scopus rating (2001): SJR 1.139 SNIP 0.952
Web of Science (2001): Indexed yes

Scopus rating (2000): SJR 1.19 SNIP 0.935
Web of Science (2000): Indexed yes

Scopus rating (1999): SJR 0.904 SNIP 0.885

Original language: English
Magnetocaloric effect, Hysteresis, Phase transition, Manganites
DOIs:
10.1016/j.jmmm.2016.05.011
Advanced Materials for High-Temperature PEM Fuel Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Hjuler, H. A. (Ekstern), Kerr, R. (Ekstern), Steenberg, T. (Ekstern), Terkelsen, C. (Ekstern), Jensen, J. O. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 127806948
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Advanced materials for polymer electrolyte membrane fuel cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Pages: 363-383
Publication date: 2016

Host publication information
Title of host publication: Electrochemical Energy: Advanced Materials and Technologies
Place of publication: Boca Raton
Publisher: C R C Press LLC
ISBN (Print): 978-1-4822-2727-7
ISBN (Electronic): 978-1-4822-2728-4
Series: Electrochemical Energy Storage and Conversion
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2016

A high mobility two-dimensional electron gas at the CaZrO3/SrTiO3 heterointerface

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern), Trier, F. (Intern), Christensen, D. V. (Intern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from TO-BE Spring Meeting 2016, Warwick, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions: A_high_mobility.pdf
Source: PublicationPreSubmission
Source-ID: 127745436
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Al-doped ZnO: RF- or DC-sputtering?

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Capres A/S, Technical University of Denmark
All Metal Organic Deposited High-Tc Superconducting Transition Edge Bolometer on Yttria-Stabilized Zirconia Substrate

We report on the results of a YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) superconductive transition edge bolometer (TEB) fabricated on a Ce$_{0.5}$La$_{0.1}$O$_{2-\delta}$ (CLO) buffered single crystalline yttria-stabilized zirconia (YSZ) substrate. Metal organic deposition was used for the fabrication of both the YBCO thin film as well as CLO buffer layer, while standard photolithography was applied for TEB preparation. YBCO thin film properties were analysed using scanning electron microscopy (SEM), X-ray diffraction (XRD), AC susceptibility and resistance versus temperature measurements. Optical response of the TEB in terms of voltage amplitude and phase was analysed and measured through four-probe technique in a liquid nitrogen cooling system. An increase in voltage amplitude response was observed for the fabricated YBCO/CLO/YSZ bolometer compared to previously reported TEBs with similarly deposited YBCO thin film on a SrTiO$_3$ (STO). This increase is assumed to be a result of the lower thermal conductivity and lower specific heat capacity of YSZ compared to STO substrate.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Sharif University of Technology
Authors: Mohajeri, R. (Ekstern), Opata, Y. A. (Intern), Wulff, A. C. (Intern), Grivel, J. (Intern), Fardmanesh, M. (Ekstern)
Number of pages: 6
Pages: 1981-1986
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Superconductivity and Novel Magnetism
Volume: 30
Issue number: 7
ISSN (Print): 1557-1939
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.91 SJR 0.34 SNIP 0.546
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.325 SNIP 0.556 CiteScore 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.384 SNIP 0.637 CiteScore 0.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.326 SNIP 0.666 CiteScore 0.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.42 SNIP 0.51 CiteScore 0.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
All-solid-state lithium-sulfur battery based on a nanoconfined LiBH₄ electrolyte

In this work we characterize all-solid-state lithium-sulfur batteries based on nano-confined LiBH₄ in mesoporous silica as solid electrolytes. The nano-confined LiBH₄ has fast ionic lithium conductivity at room temperature, 0.1 mScm⁻¹, negligible electronic conductivity and its cationic transport number (t⁺ = 0.96), close to unity, demonstrates a purely cationic conductor. The electrolyte has an excellent stability against lithium metal. The behavior of the batteries is studied by cyclic voltammetry and repeated charge/discharge cycles in galvanostatic conditions. The batteries show very good performance, delivering high capacities versus sulfur mass, typically 1220 mAhg⁻¹ after 40 cycles at moderate temperature (55°C), 0.03 C rates and working voltage of 2 V.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Utrecht University
Number of pages: 6
Pages: A2029-A2034
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 163
Issue number: 9
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.611 SNIP 1.54
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.519 SNIP 1.484
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.719 SNIP 1.706
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.962 SNIP 1.679
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.147 SNIP 1.646
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.651 SNIP 1.738
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.788 SNIP 1.708
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.657 SNIP 1.85

Original language: English
All-solid-state battery, Battery, Fast ionic conductor, Lithium sulfur battery, Solid-electrolyte
Electronic versions:
All_Solid_State_Lithium_Sulfur_Battery_Based_on_a_Nanoconfined.pdf
DOI:
10.1149/2.0771609jes

Bibliographical note
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Amino-Functional Polybenzimidazole Blends with Enhanced Phosphoric Acid Mediated Proton Conductivity as Fuel Cell Electrolytes

A new amino-functional polybenzimidazole copolymer is synthesized by homogeneous solution condensation polymerization from a novel monomer, N,N’-bis (2,4-diaminophenyl)-1,3-diaminopropane. The copolymer readily dissolves in organic solvents and shows good film forming characteristics. To balance the phosphoric acid uptake and to obtain mechanically robust membranes, the amino-functional polybenzimidazole derivative is blended with high molecular weight poly [2,2’-(m-phenylene)-5,5’-bisbenzimidazole] at different ratios. Due to the high acid uptake, the homogenous blend membranes show enhanced proton conductivity at temperatures well above 100 °C as also confirmed by the fuel cell polarization data.
An Ag based brazing system with a tunable thermal expansion for the use as sealant for solid oxide cells

An Ag-Al2TiO5 composite braze was developed and successfully tested as seal for solid oxide cells. The thermo-mechanical properties of the Ag-Al2TiO5 system and the chemical compatibility between this composite braze and relevant materials used in stacks were characterized and the leak rates as a function of the operation temperature were measured. The thermal expansion coefficient in the Ag-Al2TiO5 system can be tailored by varying the amount of the ceramic filler. The brazing process can be carried out in air, the joining partners showed a good chemical stability and sufficient low leak rates were demonstrated. Furthermore, the long-term stability of the Ag-Al2TiO5 composite braze was studied under relevant SOFC and SOEC conditions. The stability of brazed Crofer/Ag-Al2TiO5/NiO-YSZ assemblies in reducing atmosphere and in pure oxygen was investigated over 500 h at 850 °C. Additionally, a cell component test was performed to investigate the durability of the Ag-Al2TiO5 seal when exposed to dual atmosphere. The seals performed well over 900 h under electrolysis operation conditions (−0.5 A cm², 850 °C), and no cell degradation related to the Ag-Al2TiO5 sealing was found, indicating that the developed braze system is applicable for the use in SOFC/SOEC stacks.

General information
State: Published
Number of pages: 12
Pages: 339-350
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 315
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Analysis and comparison of different phase shifters for Stirling pulse tube cryocooler

Investigations of phase shifters and power recovery mechanisms are of sustainable interest for developing Stirling pulse tube cryocoolers (SPTC) with higher power density, more compact design and higher efficiency. This paper investigates the phase shifting capacity and the applications of four different phase shifters, including conventional inertance tube, gas-liquid and spring-oscillator phase shifters, as well as a power recovery displacer. Distributed models based on the electro-
acoustic analogy are developed to estimate the phase shifting capacity and the acoustic power dissipation of the three phase shifters without power recovery. The results show that both gas-liquid and spring-oscillator phase shifters have the distinctive capacity of phase shifting with a significant reduction in the inertial component length. Furthermore, full distributed models of SPTCs connected with different phase shifters are developed. The cooling performance of SPTCs using all four phase shifters are presented and typical phase relations are analyzed. The comparison reveals that the power recovery displacer with a more complicated configuration provides the highest efficiency. The gas-liquid and spring-oscillator phase shifters show equivalent efficiency compared with the inertance tube phase shifter. Approximately 10–20% of the acoustic power is dissipated by the phase shifters without power recovery, while 15–20% of the acoustic power can be recovered by the power recovery displacer, leading to a maximum coefficient of performance (COP) above 0.14 at 80 K. A merit analysis is also done by presenting the pros and cons of different phase shifters.
Analysis of diverse direct arylation polymerization (DArP) conditions toward the efficient synthesis of polymers converging with stille polymers in organic solar cells

Despite the emergence of direct arylation polymerization (DArP) as an alternative method to traditional cross-coupling routes like Stille polymerization, the exploration of DArP polymers in practical applications like polymer solar cells (PSCs) is limited. DArP polymers tend to have a reputation for being marginally inferior to Stille counterparts due to the increased presence of defects that result from unwanted side reactions in direct arylation, such as unselective C-H bond activation and homocoupling. We report ten DArP protocols across the three major classes of DArP to generate poly[(2,5-bis(2-hexyldecyloxy)phenylene)-alt-(4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole)] (PPDTBT). Through evaluation of the method and resulting photophysical and electronic properties, we show not all DArP methods are suitable for generating device-quality alternating copolymers. When DArP PPDTBT was synthesized in superheated THF with Cs2CO3, neodecanoic acid, and P(o-anisyl)3, it generated polymers of exceptional quality that performed comparably to Stille counterparts in both roll coated ITO-free and spin-coated ITO devices.
An Analytical Model for the Influence of Contact Resistance on Thermoelectric Efficiency

An analytical model is presented that can account for both electrical and hot and cold thermal contact resistances when calculating the efficiency of a thermoelectric generator. The model is compared to a numerical model of a thermoelectric leg for 16 different thermoelectric materials, as well as to the analytical models of Ebling et al. (J Electron Mater 39:1376, 2010) and Min and Rowe (J Power Sour 38:253, 1992). The model presented here is shown to accurately calculate the efficiency for all systems and all contact resistances considered, with an average difference in efficiency between the numerical model and the analytical model of -0.07 ± 0.35pp. This makes the model more accurate than previously published models. The maximum absolute difference in efficiency between the analytical model and the numerical model is 1.14pp for all materials and all contact resistances considered.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern)
Pages: 1301-1308
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Electronic Materials
Volume: 45
Issue number: 3
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
A nanoview of battery operation

The redox-active materials in lithium-ion batteries have relatively poor electronic and ionic conduction and may experience stress from charge-discharge volume changes, so their formulation into structures with nanosized features is highly desirable. On page 566 of this issue, Lim et al. (1) characterize individual nanoparticles of the positive electrode material LiFePO$_4$ during charging and discharging. This "in operando" technique ensures that all particles experience the same voltage. The current and lithium concentration are then inferred for individual particles via the change in Fe oxidation state measured during the transformation from LiFePO$_4$ to FePO$_4$ and back.
An axisymmetrical non-linear finite element model for induction heating in injection molding tools
To analyze the heating and cooling phase of an induction heated injection molding tool accurately, the temperature dependent magnetic properties, namely the non-linear B-H curves, need to be accounted for in an induction heating simulation. Hence, a finite element model has been developed, including the non-linear temperature dependent magnetic data described by a three-parameter modified Frohlich equation fitted to the magnetic saturation curve, and solved with an iterative procedure. The numerical calculations are compared with experiments conducted with two types of induction coils, built in to the injection molding tool. The model shows very good agreement with the experimental temperature measurements. It is also shown that the non-linearity can be used without the temperature dependency in some cases, and a proposed method is presented of how to estimate an effective linear permeability to use with simulation codes not able to utilize a non-linear solver. (C) 2015 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Guerrier, P. (Intern), Nielsen, K. K. (Intern), Menotti, S. (Intern), Hattel, J. H. (Intern)
Number of pages: 10
Pages: 1-10
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Finite Elements in Analysis and Design
Volume: 110
ISSN (Print): 0168-874X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.137 SNIP 1.664 CiteScore 2.39
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.246 SNIP 1.694 CiteScore 2.27
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.28 SNIP 2.052 CiteScore 2.27
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.047 SNIP 1.662 CiteScore 1.85
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.944 SNIP 2.114 CiteScore 1.7
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.767 SNIP 1.618 CiteScore 1.43
BFI (2010): BFI-level 1
An Electrochemical Impedance Spectroscopy Study on the Effects of the Surface- and Solution-Based Mechanisms in Li-O₂ Cells

The maximum discharge capacity in non-aqueous Li-O₂ batteries has been limited to a fraction of its theoretical value, largely due to a conformal deposition of Li₂O₂ on the cathode surface. However, it has recently been established that additives that increase the shielding of either O₂⁻ or Li⁺ will activate the formation of toroidal shaped Li₂O₂, thereby dramatically increasing cell capacity. Here we apply porous electrode theory to electrochemical impedance measured at the Li-O₂ cathode to investigate changes in the surface- and ionic resistance within the pores under conditions where either the surface-mechanism or the solution-mechanism is favored. Our experimental observations show that (i) an additional charge transfer process is observed in the impedance spectrum where the solution-based mechanism is favored; (ii) that the changes in the ionic resistance in the cathode during discharge (related to Li₂O₂ build up) is much greater in cells where the solution-based mechanism is activated and can qualitatively determine the extent of discharge product deposited within the pores of the cathode versus the deposition extent at the electrode/electrolyte interface; and (iii) that the observed “sudden-death” during discharge is a consequence of the increasing charge transfer resistance regardless of whether Li₂O₂ forms predominantly through either the surface- or solution-based mechanism.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, University of California
Authors: Knudsen, K. B. (Intern), Vegge, T. (Intern), McCloskey, B. D. (Ekstern), Hjelm, J. (Intern)
Number of pages: 7
Pages: A2065-A2071
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of the Electrochemical Society
Volume: 163
Issue number: 9
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Battery, Capacitance, Electrochemical impedance spectroscopy, Impedance, Li-air, Li-O2, Li2O2, Oxygen reduction, Pore clogging

Electronic versions:
An_Electrochemical_Impedance_Spectroscopy_Study_on_the_Effects_of_the_Surface_and_Solution_Based_Mechanisms_in_Li_O2Cells.pdf

DOIs:
10.1149/2.1111609jes

Bibliographical note
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An Electrochemical Impedance Study of the Capacity Limitations in Na–O2 Cells

Electrochemical impedance spectroscopy, pressure change measurements, and scanning electron microscopy were used to investigate the nonaqueous Na–O2 cell potential decrease and rise (sudden deaths) on discharge and charge, respectively. To fit the impedance spectra from operating cells, an equivalent circuit model was used that takes into account the porous nature of the positive electrode and is able to distinguish between the electrolyte resistance in the pores and the charge-transfer resistance of the pore walls. The results obtained indicate that sudden death on discharge is caused by, depending on the current density, either accumulation of large NaO2 crystals that eventually block the electrode surface and/or a thin film of NaO2 forming on the cathode surface at the end of discharge, which limits charge-transfer. The commonly observed sudden rise in potential toward the end of charge may be caused by a concentration depletion of NaO2 dissolved in the electrolyte near the cathode surface and/or an accumulation of degradation products on the cathode surface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, University of California, Stanford University
Authors: Knudsen, K. B. (Intern), Nichols, J. E. (Ekstern), Vegge, T. (Intern), Luntz, A. C. (Ekstern), McCloskey, B. D. (Ekstern), Hjelm, J. (Intern)
Pages: 10799–10805
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 120
Issue number: 20
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
An Organic Mixed Ion-Electron Conductor for Power Electronics

A mixed ionic–electronic conductor based on nanofibrillated cellulose compositad with poly(3,4-ethylene-dioxythio-phen):poly(styrene-sulfonate) along with high boiling point solvents is demonstrated in bulky electrochemical devices. The high electronic and ionic conductivities of the resulting nanopaper are exploited in devices which exhibit record values for the charge storage capacitance (1F) in supercapacitors and transconductance (1S) in electrochemical transistors.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linköping University, Innventia AB, University of Kentucky, KTH - Royal Institute of Technology
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Science
Volume: 3
Issue number: 2
Article number: 1500305
Ratings:
Scopus rating (2016): CiteScore 1.66 SJR 0.947 SNIP 0.354
Original language: English
Electronic versions:
Malti_et_al_2015_Advanced_Science.pdf
DOIs:
10.1002/advs.201670006

Bibliographical note
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Source: FindIt
Source-ID: 2292086905
Publication: Research - peer-review › Journal article – Annual report year: 2017
An Organic Mixed Ion–Electron Conductor for Power Electronics

A mixed ionic–electronic conductor based on nanofibrillated cellulose composited with poly(3,4-ethylene-dioxythio-phene):poly(styrene-sulfonate) along with high boiling point solvents is demonstrated in bulky electrochemical devices. The high electronic and ionic conductivities of the resulting nanopaper are exploited in devices which exhibit record values for the charge storage capacitance (1F) in supercapacitors and transconductance (1S) in electrochemical transistors.

A platinum-free oxygen reduction catalyst by a one-step pyrolysis process

A platinum-free oxygen reduction catalyst by a one-step pyrolysis process

Approaches to a platinum free oxygen reduction catalyst for PEM fuel cells

Approaches to a platinum free oxygen reduction catalyst for PEM fuel cells
A regenerative elastocaloric heat pump
A large fraction of global energy use is for refrigeration and air-conditioning, which could be decarbonized if efficient renewable energy technologies could be found. Vapour-compression technology remains the most widely used system to move heat up the temperature scale after more than 100 years; however, caloric-based technologies (those using the magnetocaloric, electrocaloric, barocaloric or elastocaloric effect) have recently shown a significant potential as alternatives to replace this technology due to high efficiency and the use of green solid-state refrigerants. Here, we report a regenerative elastocaloric heat pump that exhibits a temperature span of 15.3K on the water side with a corresponding specific heating power up to 800Wkg\(^{-1}\) and maximum COP (coefficient-of-performance) values of up to 7. The efficiency and specific heating power of this device exceeds those of other devices based on caloric effects. These results open up the possibility of using the elastocaloric effect in various cooling and heat-pumping applications.

Assessment of potential biomass energy production in China towards 2030 and 2050
The objective of this paper is to provide a more detailed picture of potential biomass energy production in the Chinese energy system towards 2030 and 2050. Biomass for bioenergy feedstocks comes from five sources, which are agricultural crop residues, forest residues and industrial wood waste, energy crops and woody crops, animal manure, and municipal solid waste. The potential biomass production is predicted based on the resource availability. In the process of identifying biomass resources production, assumptions are made regarding arable land, marginal land, crops yields, forest growth rate, and meat consumption and waste production. Four scenarios were designed to describe the potential biomass energy production to elaborate the role of biomass energy in the Chinese energy system in 2030. The assessment shows that under certain restrictions on land availability, the maximum potential biomass energy productions are estimated to be 18,833 and 24,901 PJ in 2030 and 2050.
A stability study of polymer solar cells using conjugated polymers with different donor or acceptor side chain patterns

Improvement of the power conversion efficiency and long term stability remains to be of crucial importance for the further development of polymer solar cells (PSCs). Herein, a donor-acceptor copolymer based on 4,8-di((thiophene-2-y1)benzo[1,2-b:4,5-b']dithiophene (DTBDT) and 4,7-di((thiophene-2-y1)benzo[c][1,2,5]thiadiazole (DTBT), specifically selected because of its suitability for roll-coating in the ambient environment, is investigated in terms of operational stability via partial exchange (5 or 10%) of the alkyl side chain on either the donor or the acceptor monomer with a 2-
hydroxyethyl or 2-phenylethyl group. It is shown that the exchange of the hexyl chain on the DTBT moiety has a negative impact on the stability of the polymer as well as on the performance of the resulting PSCs. On the other hand, partial exchange of the 2-hexyldecyl side chain of the BDT unit by a 2-hydroxyethyl group results in an improved photochemical stability of the polymer film and a higher efficiency of 5.6% for the spin-coated PSC. The stability of roll-coated devices also slightly increases with the incorporation of 10% of either the 2-hydroxyethyl or 2-phenylethyl side chain.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Hasselt University, Vrije Universiteit Brussel
Authors: Heckler, I. M. (Intern), Kesters, J. (Ekstern), Defour, M. (Ekstern), Penxten, H. (Ekstern), Van Mele, B. (Ekstern), Maes, W. (Ekstern), Bundgaard, E. (Intern)
Number of pages: 13
Pages: 16677-16689
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Materials Chemistry A
Volume: 4
Issue number: 42
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
DOI: 10.1039/c6ta07244e
Source: Findit
Source-ID: 2347360693
Publication: Research - peer-review › Journal article – Annual report year: 2016

**A systematic approach applied in design of a micro heat exchanger**

The number of products benefiting from micro components in the market is increasing, and consequently, the demand for well-matched tools, equipment and systems with micro features is eventually increasing as well. During the design process of micro products, a number of issues appear which are inherent due to the down scaling or physical phenomena dominating in the micro range but negligible in the macro scale. In fact, some aspects in design for micro manufacturing are considerably different compared to the design procedure taken at the macro level. Identifying the differences between design considerations at micro compared to macro scale, and defining potential guidelines based on them, provides an opportunity to modify the conventional design methodologies towards becoming micro specific. In this paper, the need for a micro-oriented approach for designing micro products which has not been investigated hitherto studied. For this purpose, an additional step named “Rules To Consider” (RTC) is added to the conventional design methodologies. This step is constituted based on the feedbacks gained during analyzing the different iterations of the design. The knowledge obtained during the design process of a micro product can be added to the RTC unit, and this unit becomes enriched progressively in design process of similar micro products and supplemented to the conventional design methodologies to be served as a micro-oriented design methodology. In order to present the application of RTC unit, the design process of a micro heat exchanger is investigated. Manufacturability and functional performance are considered as evaluation criteria, and the lessons learned from each design iteration and evaluation are employed in the subsequent design proposals until an acceptable design is achieved. Thermal performance of the heat exchangers is evaluated using finite element (FE) simulation of the conjugate heat transfer. The design proposals are optimized in terms of geometrical
dimensions, and a sensitivity analysis is conducted on the mass flow rate and heat generation power in the heat source. Finally, the designs with higher thermal performance and manufacturability are introduced. The result of the thermal analysis reveals the fact that the presence of the fins and modification of their dimensions as well as the constituent material for fabricating the micro heat exchanger do not significantly improve the thermal performance of the micro heat exchangers. This is an interesting outcome which can result in considerable reduction of the manufacturing costs by simplifying the geometrical design of the heat exchanger. The micro-specific design considerations which are extracted from the design process of the micro heat exchanger are added to the RTC unit and can be applied as guidelines in design process of any other micro heat exchanger. In other words, the current study can provide a useful guideline in design for manufacturing of micro products.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Management Engineering, Department of Energy Conversion and Storage
Authors: Omidvarnia, F. (Intern), Hansen, H. N. (Intern), Sarhadi, A. (Intern)
Number of pages: 9
Pages: 1187-1195
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Advanced Manufacturing Technology
Volume: 82
Issue number: 5
ISSN (Print): 0268-3768
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.3 SJR 0.967 SNIP 1.548
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.858 SNIP 1.274 CiteScore 1.8
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.084 SNIP 1.879 CiteScore 2.03
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.133 SNIP 2.117 CiteScore 2.26
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.982 SNIP 2.091 CiteScore 1.75
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.821 SNIP 1.624 CiteScore 1.61
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.777 SNIP 1.418
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.806 SNIP 1.355
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 0.509 SNIP 1.011
A TEM study of morphological and structural degradation phenomena in LiFePO$_4$-CB cathodes: Morphological and structural degradation in LiFePO$_4$-CB cathodes

LiFePO$_4$-based cathodes suffer from various degradation mechanisms, which influences the battery performance. In this paper, morphological and structural degradation phenomena in laboratory cathodes made of LiFePO$_4$ mixed with carbon black (CB) in a 1 mol/L LiPF$_6$ in EC: DMC (1:1 by weight) electrolyte are investigated by transmission electron microscopy at various preparation, assembling, storage, and cycling stages. High-resolution transmission electron microscopy imaging shows that continuous SEI layers are formed on the LiFePO$_4$ particles and that both storage and cycling affect the formation. Additionally, loss of CB crystallinity, CB aggregation, and agglomeration is observed. Charge–discharge curves and impedance spectra measured during cycling confirm that these degradation mechanisms reduce the cathode conductivity and capacity.

General information
State: published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Ngo, D. (Intern), Scipioni, R. (Intern), Simonsen, S. B. (Intern), Jørgensen, P. S. (Intern), Jensen, S. H. (Intern)
Number of pages: 11
Pages: 2022-2032
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Energy Research
Volume: 40
Issue number: 14
ISSN (Print): 0363-907X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.44 SJR 0.739 SNIP 0.857
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.917 SNIP 1.066 CiteScore 2.52
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.06 SNIP 1.35 CiteScore 2.56
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.068 SNIP 1.65 CiteScore 2.71
ISI indexed (2013): ISI indexed yes
A thermoelectric power generating heat exchanger: Part I – Experimental realization

An experimental realization of a heat exchanger with commercial thermoelectric generators (TEGs) is presented. The power producing capabilities as a function of flow rate and temperature span are characterized for two different commercial heat transfer fluids and for three different thermal interface materials. The device is shown to produce 2W per TEG or 0.22W cm⁻² at a fluid temperature difference of 175 °C and a flow rate per fluid channel of 5 L min⁻¹. One experimentally realized design produced 200W in total from 100 TEGs. For the design considered here, the power production is shown to depend more critically on the fluid temperature span than on the fluid flow rate. Finally, the temperature span across the TEG is shown to be 55–75% of the temperature span between the hot and cold fluids. © 2016 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Peltpower ApS
Authors: Bjørk, R. (Intern), Sarhadi, A. (Intern), Pryds, N. (Intern), Lindeburg, N. (Ekstern), Viereck, P. (Ekstern)
Pages: 473–480
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Conversion and Management
Volume: 119
ISSN (Print): 0196-8904
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.04 SJR 2.287 SNIP 2.065
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.09 SNIP 2.092 CiteScore 5.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.854 SNIP 2.835 CiteScore 5.35
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.669 SNIP 2.558 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 2.277 CiteScore 3.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.292 SNIP 1.846 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.75
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.339 SNIP 1.797
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.508 SNIP 1.905
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.196 SNIP 1.811
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.327 SNIP 1.816
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.577 SNIP 1.799
Scopus rating (2004): SJR 1.049 SNIP 1.466
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.903 SNIP 1.321
Scopus rating (2002): SJR 1.089 SNIP 1.463
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.81 SNIP 0.855
Scopus rating (2000): SJR 0.576 SNIP 0.688
Scopus rating (1999): SJR 0.515 SNIP 0.724
Original language: English
Thermoelectric, Heat exchanger, Power generation, Heat transfer fluid, Thermal interface
DOIs:
10.1016/j.enconman.2016.04.042
Source: PublicationPreSubmission
Source-ID: 123614797
Publication: Research - peer-review › Journal article – Annual report year: 2016
A thermoelectric power generating heat exchanger: Part II – Numerical modeling and optimization

In Part I of this study, the performance of an experimental integrated thermoelectric generator (TEG)-heat exchanger was presented. In the current study, Part II, the obtained experimental results are compared with those predicted by a finite element (FE) model. In the simulation of the integrated TEG-heat exchanger, the thermal contact resistance between the TEG and the heat exchanger is modeled assuming either an ideal thermal contact or using a combined Cooper–Mikic–Yovanovich (CMY) and parallel plate gap formulation, which takes into account the contact pressure, roughness and hardness of the interface surfaces as well as the air gap thermal resistance at the interface. The combined CMY and parallel plate gap model is then further developed to simulate the thermal contact resistance for the case of an interface material. The numerical results show good agreement with the experimental data with an average deviation of 17% for the case without interface material and 12% in the case of including additional material at the interfaces. The model is then employed to evaluate the power production of the integrated system using different interface materials, including graphite, aluminum (Al), tin (Sn) and lead (Pb) in a form of thin foils. The numerical results show that lead foil at the interface has the best performance, with an improvement in power production of 34% compared to graphite foil. Finally, the model predicts that for a certain flow rate, increasing the parallel TEG channels for the integrated systems with 4, 8, and 12TEGs enhances the net power per TEG with average values of 2.5%, 3% and 5%, respectively.

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General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Peltpower ApS
Authors: Sarhadi, A. (Intern), Bjørk, R. (Intern), Lindeburg, N. (Ekstern), Viereck, P. (Ekstern), Pryds, N. (Intern)
Pages: 481–487
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Conversion and Management
Volume: 119
ISSN (Print): 0196-8904
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.04 SJR 2.287 SNIP 2.065
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.09 SNIP 2.092 CiteScore 5.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.854 SNIP 2.835 CiteScore 5.35
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.669 SNIP 2.558 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 2.277 CiteScore 3.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.292 SNIP 1.846 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.75
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.339 SNIP 1.797
Web of Science (2009): Indexed yes
Attempts at doping indium in MgB₂

Indium (In) doped MgB₂ polycrystalline samples were prepared by solid-liquid phase reaction in Ar. After reaction at 800 °C, less than 1 at. % Mg was replaced by In in the MgB₂ phase, without significant influence on its lattice parameters and only a slight decrease of its superconducting transition temperature. For all studied In concentrations in the nominal composition, the formation of InMg was evidenced by X-ray diffraction. The critical current density and accommodation field of the wires are decreased in the samples containing In. The flux pinning mechanism can be described by surface pinning in both the doped and undoped samples.
A Two-Level Undercut-Profile Substrate for Chemical-Solution-Based Filamentary Coated Conductors

A recently developed two-level undercut-profile substrate (2LUPS), containing two levels of plateaus connected by a curved wall with an undercut profile, enables self-forming filaments in a coated conductor during physical line-of-sight deposition of buffer and superconducting layers. In the present study, the 2LUPS concept is applied to a commercial cube-textured Ni-5at.% W tape, and the surface of the 2LUPS coated with two Gd$_2$Zr$_2$O$_7$ buffer layers using chemical solution deposition is examined. Except for narrow regions near the edge of upper plateaus, the plateaus are found to be covered by strongly textured Gd$_2$Zr$_2$O$_7$ buffer layers after dip coating and sintering.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization, SUBRA IVS, Sharif University of Technology
Authors: Wulff, A. C. (Intern), Lundeman, J. H. (Ekstern), Hansen, J. B. (Ekstern), Mishin, O. (Intern), Yue, Z. (Intern), Mohajeri, R. (Ekstern), Grivel, J. (Intern)
Number of pages: 4
Publication date: 2016
A viable electrode material for use in microbial fuel cells for tropical regions

Electrode materials are critical for microbial fuel cells (MFC) since they influence the construction and operational costs. This study introduces a simple and efficient electrode material in the form of palm kernel shell activated carbon (AC) obtained in tropical regions. The novel introduction of this material is also targeted at introducing an inexpensive and durable electrode material, which can be produced in rural communities to improve the viability of MFCs. The maximum voltage and power density obtained (under 1000 Ω load) using an H-shaped MFC with AC as both anode and cathode electrode material was 0.66 V and 1.74 W/m3, respectively. The power generated by AC was as high as 86% of the value obtained with the extensively used carbon paper. Scanning electron microscopy and Denaturing Gradient Gel Electrophoresis (DGGE) analysis of AC anode biofilms confirmed that electrogenic bacteria were present on the electrode surface for substrate oxidation and the formation of nanowires.
Baselines for Lifetime of Organic Solar Cells

The process of accurately gauging lifetime improvements in organic photovoltaics (OPVs) or other similar emerging technologies, such as perovskites solar cells, is still a major challenge. The presented work is part of a larger effort of developing a worldwide database of lifetimes that can help establishing reference baselines of stability performance for OPVs and other emerging PV technologies, which can then be utilized for pass-fail testing standards and predicting tools. The study constitutes scanning of literature articles related to stability data of OPVs, reported until mid-2015 and collecting the reported data into a database. A generic lifetime marker is utilized for rating the stability of various reported devices. The collected data is combined with an earlier developed and reported database, which was based on articles reported until mid-2013. The extended database is utilized for establishing the baselines of lifetime for OPVs tested under different conditions. The work also provides the recent progress in stability of unencapsulated OPVs with different architectures, as well as presents the updated diagram of the reported record lifetimes of OPVs. The presented work is another step forward towards the development of pass-fail testing standards and lifetime prediction tools for emerging PV technologies.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Functional organic materials, ICFO - Institute of Photonic Sciences, University of Minho, Zurich University of Applied Sciences, CNRS, Institut Català de Nanociència i Nanotecnologia, Technische Universität Ilmenau, Cyprus University of Technology, Imperial College London
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 6
Issue number: 22
Article number: 1600910
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.124 SNIP 2.045
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Degradation, Lifetime baseline, Lifetime database, Organic photovoltaics

Beneficial Effect of Surface Decorations on the Surface Exchange of Lanthanum Strontium Ferrite and Dual Phase Composites

Perovskites within the (La,Sr)(Fe,Co)O₃ class of materials show variations in the oxygen stoichiometry depending on temperature and oxygen activity and can potentially be used as catalysts, electrodes in high-temperature solid oxide fuel cells, gas sensors or for oxygen transport membranes. These perovskites possess a mixed ionic and electronic conductivity (MIEC), which can be highly beneficial for the processes on oxygen electrode surfaces. The oxygen transport through a MIEC is determined by the rate of the oxygen exchange over the gas-solid interface and the diffusivity of oxide ions and electrons (or holes) in the bulk. The oxygen exchange process over the surface in general involves several reaction steps, O₂ adsorption, dissociation, charge transfer and incorporation of ionic species. The Co-free end member of the material class, LSF (e.g. (La0.6Sr0.4FeO₃-δ) is fairly low cost and chemically stable in both mildly reducing and oxidizing atmosphere. The electronic conductivity is excellent (283 S/cm at 800 °C) but the ionic conductivity especially at low temperature is limited (0.014 S/cm, 800 °C). Due to these properties the material is a candidate for use in composite membranes in combination with a better ionic conducting material like CGO. Such systems are also excellent model systems for fundamental studies of the oxygen exchange process.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Twente
Authors: Ovtar, S. (Intern), Søgaard, M. (Intern), Song, J. (Ekstern), Hendriksen, P. V. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
abstract2.pdf
Links:
http://ma.ecsdl.org/content/MA2016-02/48/3575.abstract
Source: PublicationPreSubmission
Source-ID: 126931726
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Benefits of Integrating Geographically Distributed District Heating Systems

General information
State: Published
Benefits of Integrating Geographically Distributed District Heating Systems

Although liberalization of the electricity day-ahead markets has gained pace throughout the Europe, district heating markets are often dominated by lack of competition between suppliers, which curbs the potential of having cheaper systems in terms of socio-economic costs, and technically better system in terms of CO2 emissions. In order to assess the financial and technical outcome of connecting five adjacent district heating systems, a linear continuous optimization model that minimizes total socio-economic costs was developed. Geographical distribution of different district heating systems was truly represented. The model was adapted to the case of Sønderborg municipality in Denmark and the results show that three out of four interconnections are economic feasible in the present system. In the reference year (2013) total system costs were 4.1 % lower, while total primary energy supply was reduced by 1.76 %. For the year 2029, in which intermittent renewable energy sources are dominating the energy generation, total socio-economic costs were reduced by 5.9 %, CO2 emissions by 7.1 % and primary energy supply by 8.4 % after the adjacent district heating systems were connected. Hence, the integration of district heating systems have beneficial impact on the integration of intermittent renewable energy sources.
Biogas Catalytic Reforming Studies on Nickel-Based Solid Oxide Fuel Cell Anodes

Heterogeneous catalysis studies were conducted on two crushed solid oxide fuel cell (SOFC) anodes in fixed-bed reactors. The baseline anode was Ni/ScYSZ (Ni/scandia and yttria stabilized zirconia), the other was Ni/ScYSZ modified with Pd/doped ceria (Ni/ScYSZ/Pd-CGO). Three main types of experiments were performed to study catalytic activity and effect of sulfur poisoning: (i) CH4 and CO2 dissociation; (ii) biogas (60% CH4 and 40% CO2) temperature-programmed reactions (TPRxn); and (iii) steady-state biogas reforming reactions followed by postmortem catalyst characterization by temperature-programmed oxidation and time-of-flight secondary ion mass spectrometry. Results showed that Ni/ScYSZ/Pd-CGO was more active for catalytic dissociation of CH4 at 750°C and subsequent reactivity of deposited carbonaceous species. Sulfur deactivated most catalytic reactions except CO2 dissociation at 750°C. The presence of Pd-CGO helped to mitigate sulfur deactivation effect; e.g. lowering the onset temperature (up to 190°C) for CH4 conversion during temperature-programmed reactions. Both Ni/ScYSZ and Ni/ScYSZ/Pd-CGO anode catalysts were more active for dry reforming of biogas than they were for steam reforming. Deactivation of reforming activity by sulfur was much more severe under steam reforming conditions than dry reforming; a result of greater sulfur retention on the catalyst surface during steam reforming.
Can We Replace Platinum Metals in PEM Fuel Cells and Electrolyzers?

General information
State: Published
Capturing metal-support interactions in situ during the reduction of a Re promoted Co/γ-Al₂O₃ catalyst

The reduction of a Re promoted Co/γ-Al₂O₃ catalyst was monitored in situ by synchrotron X-ray powder diffraction (XRPD) under H₂ environment. Whole powder pattern analysis revealed a non-linear expansion of the unit cell of γ-Al₂O₃ during the reduction process, suggesting the diffusion of Co cations into the structure of the support. The non-linear cell expansion coincided with the formation of a CoO phase. In addition, space resolved diffraction at the inlet and the outlet of the reactor evidenced a negative effect of the partial pressure of indigenous H₂O(g) on the reduction process.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, European Synchrotron Radiation Facility, Norwegian University of Science and Technology, SINTEF
Authors: Tsakoumis, N. E. (Ekstern), Johnsen, R. E. (Intern), van Beek, W. (Ekstern), Rønning, M. (Ekstern), Rytter, E. (Ekstern), Holmen, A. (Ekstern)
Number of pages: 4
Pages: 3239-3242
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Communications
Volume: 52
Issue number: 15
ISSN (Print): 1359-7345
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.506 SNIP 1.159
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.664 SNIP 1.314 CiteScore 6.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.701 SNIP 1.446 CiteScore 6.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.755 SNIP 1.38 CiteScore 6.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.09 SNIP 1.347 CiteScore 6.21
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.857 SNIP 1.322 CiteScore 5.96
ISI indexed (2011): ISI indexed yes
To solve issues of coking and redox instability related to the presence of nickel in typical fuel electrodes in solid oxide cells, Gd-doped CeO$_2$ (CGO) electrodes were studied using symmetric cells. These electrodes showed high electro-catalytic activity, but low electronic conductivity. When infiltrated with Sr$_{0.99}$Fe$_{0.75}$Mo$_{0.25}$O$_{3-\delta}$ (SFM), the electronic conductivity was enhanced. However, polarization resistance of the cells increased, suggesting that the infiltrated material is less electro-catalytically active and was partly blocking the CGO surface reaction sites. The activity could be regained by infiltrating nano-sized CGO or NiCGO on top of SFM, while still sustaining the high electronic conductivity. Ohmic resistance of the electrodes was thus practically eliminated and performance comparable to, or better than, state-of-the-art fuel electrodes was achieved. The Ni-containing cells were damaged by carbon deposition in a CO/CO$_2$-atmosphere, while none of the non-nickel cells catalyzed carbon. Stability towards redox cycles was also proven.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Haldor Topsoe AS
Authors: Skafte, T. L. (Intern), Sudireddy, B. R. (Intern), Blennow, P. (Ekstern), Graves, C. R. (Intern)
Number of pages: 14
Pages: 201-214
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: E C S Transactions
Volume: 72
Issue number: 7
Ceramic tape casting: A review of current methods and trends with emphasis on rheological behaviour and flow analysis

Tape casting has been used to produce thin layers of ceramics that can be used as single layers or can be stacked and laminated into multilayered structures. Today, tape casting is the basic fabrication process that provides multilayered capacitors and multilayered ceramic packages. In tape casting the rheological behaviour of the slurry as well as the material flow during casting are of utmost importance since these phenomena to a large extent determine the final properties and hence the quality of the cast product. During the last decades this has led to an increasing number of works in literature within fluid flow analysis of tape casting. In the present paper a review of the development of the tape casting process with particular focus on the rheological classifications as well as modelling the material flow is hence presented and in this context the current status is examined and future potential discussed.

General information

State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Electrofunctional materials, Nanyang Technological University, National Technical University of Athens
Authors: Jabbaribehnam, M. (Intern), Bulatova, R. (Intern), Tok, A. I. Y. (Ekstern), Bahl, C. (Intern), Mitsoulis, E. (Ekstern), Hattel, J. H. (Intern)
Pages: 39-61
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Materials Science and Engineering B: Advanced Functional Solid-state Materials
Volume: 212
Challenges in going from 2nd order to 1st order materials in magnetic refrigeration devices

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Number of pages: 1
Publication date: 2016
Challenges in Membrane Electrode Assembly Technologies

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Bibliographical note
Invited plenary talk
Organisation: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Characterisation of a Planar Solid Oxide Cell Stack Operated at Elevated Pressure

As the global and local energy production becomes more dependent on intermittent renewable sources like wind and solar, efficient and reversible conversion of electricity to storable fuels becomes increasingly important. Solid oxide cells (SOCs) are interesting in this context since they can be operated either as electrolyser (SOEC) to convert electricity to fuels such as hydrogen or methane, and as fuel cells (SOFC) to convert fuels to electricity. Both productivity and conversion efficiency can be improved if the SOC operation pressure can be increased from ambient pressure to 10-30 bar.

Here we characterize an SOC stack operated at pressures from ambient pressure to 10 bar without fluctuations in the steam supply. The pressure dependency of stack temperature, cell area specific resistance (ASR), current-voltage (iV) curves, stack impedance spectra and pressure drop across the stack and heat exchangers is analyzed and the expected impact of pressurization on the hydrogen production cost is evaluated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Haldor Topsoe AS
Authors: Jensen, S. H. (Intern), Graves, C. R. (Intern), Chen, M. (Intern), Sun, X. (Intern), Hansen, J. B. (Ekstern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3077
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/40/3077.abstract?sid=92d73baa-3694-4497-ad3b-bfb3b4013b9b
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Characterization and modeling of organic (P3HT:PCBM) solar cells as a function of bias and illumination

We investigated the response of roll coated organic solar cells at different bias voltages and illumination levels to implement a detailed impedance model. The technique used for the investigation is based on the combination of standard DC characterization with the impedance spectroscopy at different bias and illumination intensity conditions. We analyzed both fresh and intentionally degraded cells. The impedance spectra show different peaks evolutions, depending on the
degradation of the cells. Moreover, the same trend appears by measuring the cell at different illumination levels. To describe the cell impedance behaviors we suggest an electrical model based on distributed elements. By fitting the model to experimental data, we extrapolate the parameters related to electron transport, recombination and accumulation. The main differences between fresh and degraded samples are underlined. (C) 2016 Elsevier B.V. All rights reserved.

General information
State: Published
Number of pages: 9
Pages: 337-345
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 157
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.524 SNIP 2.121
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.991 SNIP 1.977
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.654 SNIP 1.458
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.359 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.447 SNIP 1.799
Characterization of a Planar Solid Oxide Cell Stack Operated at Elevated Pressure

As global and local energy production becomes more dependent on intermittent renewable sources like wind and solar, efficient and reversible conversion of electricity to storable fuels becomes increasingly important. Solid oxide cells (SOCs) are interesting in this context since they can be operated either as electrolyzers (SOEC) to convert electricity to fuels such as hydrogen or methane, and as fuel cells (SOFC) to convert fuels to electricity. Both productivity and conversion efficiency can be improved if the SOC operation pressure can be increased from ambient pressure to 10–30 bar. In this paper we characterize an SOC stack operated at pressures from ambient pressure to 10 bar. The pressure dependency of stack temperature, cell area specific resistance (ASR), current-voltage (IV) curves, stack impedance spectra and pressure drop across the stack and heat exchangers is analyzed in this paper. Additionally, the expected impact on the hydrogen production efficiency and cost is discussed.
Characterization Of Biaxial Strain Of Poly(L-Lactide) Tubes

Poly(L-lactide) (PLLA) in its L-form has promising mechanical properties. Being a semi-crystalline polymer, it can be subjected to strain-induced crystallization at temperatures above $T_g$ and can thereby become oriented. Following a simultaneous (SIM) biaxial strain process or a sequential (SEQ) biaxial strain process, the mechanical properties of biaxial strained tubes can be further improved. This study investigated these properties in relation to their morphology and crystal orientation. Both processes yield the same mechanical strength and modulus, yet exhibit different crystal orientation. Through further WAXS analysis it was found that the SEQ biaxial strain yields larger interplanar spacing and distorted crystals and looser packing of chains. However, this does not influence the mechanical properties negatively. A loss of orientation in SEQ biaxial strained samples at high degrees of strain was detected, but not seen for SIM biaxial strain, and did not correlate with mechanical performance in either case. However, post-annealing reduced the orientation to the same level in both cases, and the modulus and strength is decreased for both SIM and SEQ biaxial. It is therefore concluded that mechanical properties after biaxial strain are related to strain-induced amorphous orientation and the packing of crystals, rather than strain-induced crystallinity.
Renewable energies are a critical and necessary technological development deeply connected to human evolution and even survival. The extraordinary technological development of the past century brought tremendous changes to the planet which, despite the scepticism of some, are indubitably affecting the natural ecosystem and maybe even the destiny of Earth. Human evolution does not mean only advanced technological development, but also deeper consciousness and responsibility for the next generations to come. Everything on Earth exists because of the Sun: heat, wind, life... everything. Therefore, solar energy is one of the answers for renewable energy. In this thesis, the research has been conducted on polymer solar cells. In particular, the thesis deals with the extensive study of device lifetime, characterized with several methods: from bare benchmarking of the lifetimes, to more advanced characterizations of different device properties and materials under degradation. The devices were mostly produced using roll-to-roll processing, which is compatible with an upscaled production, essential for commercialization. Therefore, a fast characterization of a large number of samples has been a general goal of this thesis, which has been driving the choice of both the measurement techniques and also the methods for data handling. This included the development of both novel hardware and software. The possibility of fast screening a large number of devices can in fact lead to a faster improvement of the technology, due to the large amount of experimental data that would become available in a relatively short time. Real time in-situ data analysis, during the fabrication, is possibly the ultimate type of fast screening technique. In-situ X-ray diffraction analysis is a good example of a fast screening technique, that has been presented in this thesis. The challenge of standardizing the report of lifetime was addressed, with the development of novel methods for intercomparing the lifetime of a large amount of data. In particular, the comparison of the lifetime extracted under accelerated and outdoor conditions allowed for the generation of a tool for lifetime prediction. The lifetime extracted from outdoor conditions was found to be in between the one extracted from moderate conditions (shelf test and high temperature storage) and harsher conditions (light soaking and damp heat test). In-depth characterization techniques were also employed in order to study the effect of degradation on the device structure and its interfaces. This was done by exploiting different techniques that measured different properties of the device: mechanical, imaging, and electrical. Mechanical characterization of roll-to-roll processed samples allowed the detection of a mechanically weak interface between PEDOT:PSS and ZnO, which could be improved by applying a combination of humidity and high temperature. Moreover, impedance spectroscopy combined with modelling enabled identifying the degradation of the ZnO / active layer interface. Finally, imaging of cross sections of an ITO-free roll-to-roll processed device was performed successfully using transmission electron microscopy. The cross sections were prepared both with focused-ion-beam and ultramicrotomy, which gave the possibility for effectively comparing these two techniques. Moreover, the sectioning of the solar cells with a diamond blade, in the ultramicrotomy, opened the possibility for a fast cross sections preparation. An optimal lifetime characterization, producing relevant data for the whole OPV field, both on the macroscopic and on the microscopic level, in a fast and automatic way, is possibly the perfect lifetime characterization. The extensive characterization of lifetime performed in this thesis was done with the attempt to approach to such an optimal characterization, providing valuable results to study the effect of degradation and also providing effective tools for increasing the lifetime data exchange within the OPV research field.
Characterization of YBa$_2$Cu$_3$O$_{7-\delta}$ Films With Various Porous Structures Grown by Metalorganic Decomposition Route

Metalorganic decomposition route with trifluoroacetates has been successfully used to fabricate YBa2Cu3O7−δ (YBCO)-based coated conductors with an excellent performance. The microstructure and superconducting properties of YBCO films were controlled by the substrate properties and the solution chemistry or by regulating the processing parameters during the film heat treatment. In this work, three YBCO films with various porous structures, namely, a fully dense sample, a cell-structured sample with dense regions surrounded by a porous structure, and a highly porous sample, were deposited on single crystalline substrates (i.e., LaAlO3 and La-doped CeO2 buffered YSZ). The samples were investigated by X-ray diffraction, scanning electron microscopy, a vibrating sample magnetometer, and a magneto-optical imaging technique. All three films show highly epitaxial growth and good superconducting properties (Tc onset around 89 K and Ic higher than 3 MA/cm2 at 77 K in self-field). However, we found that the porous structures formed by different nucleation and growth mechanisms during the sintering process still have strong influence on the superconducting properties, particularly when applying magnetic fields. The pinning behaviors in the films related to the nanoporous structures, characterized by magnetic moment measurements and visualized by magneto-optical imaging, will be discussed in detail.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Oslo
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Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.431 SNIP 1.171 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Classical molecular dynamics and quantum abs-initio studies on lithium-intercalation in interconnected hollow spherical nano-spheres of amorphous Silicon

A high concentration of lithium, corresponding to charge capacity of ~4200 mAh/g, can be intercalated in silicon. Unfortunately, due to high intercalation strain leading to fracture and consequent poor cyclability, silicon cannot be used as anode in lithium ion batteries. But recently interconnected hollow nano-spheres of amorphous silicon have been found to exhibit high cyclability. The absence of fracture upon lithiation and the high cyclability has been attributed to reduction in intercalation stress due to hollow spherical geometry of the silicon nano-particles. The present work argues that the hollow spherical geometry alone cannot ensure the absence of fracture. Using classical molecular dynamics and density functional theory based simulations; satisfactory explanation to the absence of fracture has been explored at the atomic scale.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Defense Metallurgical Research Laboratory, Center for Study of Science, Technology and Policy, Indian Institute of Technology, Kharagpur
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Number of pages: 30
Pages: 165–172
Publication date: 2016
Main Research Area: Technical/natural sciences
Coatings for High Temperature Corrosion Protection of Stainless Steels

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Talić, B. (Intern), Molin, S. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Comparative Indoor and Outdoor Degradation of Organic Photovoltaic Cells via Inter-laboratory Collaboration
We report on the degradation of organic photovoltaic (OPV) cells in both indoor and outdoor environments. Eight different research groups contributed state of the art OPV cells to be studied at Pomona College. Power conversion efficiency and fill factor were determined from IV curves collected at regular intervals over six to eight months. Similarly prepared devices were measured indoors, outdoors, and after dark storage. Device architectures are compared. Cells kept indoors performed better than outdoors due to the lack of temperature and humidity extremes. Encapsulated cells performed better due to the minimal oxidation. Some devices showed steady aging but many failed catastrophically due to corrosion of electrodes not active device layers. Degradation of cells kept in dark storage was minimal over periods up to one year.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Pomona College, Heliatek GmbH, IMEC, Holst Center, Fraunhofer ISE, Ilmenau University of Technology, Universidad Autonoma de Barcelona
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Polymers
Volume: 8
Issue number: 1
Article number: 8010001
ISSN (Print): 2073-4360
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 0.96 SNIP 1.372 CiteScore 3.74
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.907 SNIP 1.345 CiteScore 3.37
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 1.114 SNIP 1.687 CiteScore 4.1
Scopus rating (2013): SJR 0.91 SNIP 1.108 CiteScore 3.1
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 0.564 SNIP 0.711 CiteScore 1.68
Comparative study of PBI Cross Linked Utilizing Agents of Varying Steric Configurations

The high thermal and chemical stability of poly[2,2’-(m-phenylene)-5,5’ bibliimidazole] (PBI) accounts for its wise spread use in high temperature polymer electrolyte membrane fuel cells (HT- PEMFC). By doping the membrane with phosphoric acid (PA) ionic conductivity is obtained. Thus conductivity is dependent on the amount of PA present within the membrane. However mechanical properties are reduced are significantly reduced due to the plasticizing effect shown by PA [1]. This effect is due to PBI chain displacement. This effect can be lessened by use of cross linking [2-4]. This can be obtained using ionic or covalent cross linking. When considering such, little attention is devoted to explore the effect of the sterical configuration of the cross linking agent.

In this contribution three different cross linking agents are utilized to evaluate how these affects final membrane properties.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
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Pages: 124-124
Publication date: 2016

Comparing superconducting and permanent magnets for magnetic refrigeration

We compare the cost of a high temperature superconducting (SC) tape-based solenoid with a permanent magnet (PM) Halbach cylinder for magnetic refrigeration. Assuming a five liter active magnetic regenerator volume, the price of each type of magnet is determined as a function of aspect ratio of the regenerator and desired internal magnetic field. It is shown that to produce a 1 T internal field in the regenerator a permanent magnet of hundreds of kilograms is needed or an area of superconducting tape of tens of square meters. The cost of cogling the SC solenoids shown to be a small fraction of the cost of the SC tape. Assuming a cost of $10000/m² of SC tape and a price of the permanent magnet of 100 $/kg, the superconducting solenoid is shown to be a factor of 0.3-3 times more expensive than the permanent magnet, for a desired field from 0.5-1.75 T and the geometrical aspect ratio of the regenerator. This factor decreases for increasing field strength, indicating that the superconducting solenoid could be suitable for high field, large cooling power applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern), Bahl, C. R. H. (Intern), Smith, A. (Intern), Wulff, A. C. (Intern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences
Comparison of the electron work function, hole concentration and exciton diffusion length for P3HT and PT prepared by thermal or acid cleavage

The electron work function, hole concentration and diffusion length were compared for poly(3-hexylthiophene) polymer (P3HT) that is commonly used for construction of solar cells, and two types of native polythiophene (PT) samples which are prospective candidates for this purpose. The polythiophene samples were prepared from 2 different precursors by thermal or chemical treatment at room temperature. Cyclic voltammetry and work function measurements were used for estimating the concentration of holes. The measured data were evaluated assuming the validity of band theory based on the tight-binding model. Published data on the valence bandwidth were used for calculating the value of the overlap integral which is related to the hole effective mass. Energy band diagrams were constructed for all 3 materials. Finally, the exciton diffusion length, which is a critical parameter for the application of conjugated polymer materials in solar cells, was measured by a modified surface photovoltage method. The approach allowed us to identify the differences in the material properties related to the processing method. Morphology of the samples determined by AFM was another tool showing these differences. It is stated that a native polythiophene prepared by treatment with acids is a prospective material for solar cells and shows a similar quality as that produced by a thermal process. © 2015 Elsevier Ltd. All rights reserved.
Comparison of ultramicrotomy and focused-ion-beam for the preparation of TEM and STEM cross section of organic solar cells

The challenge of preparing cross sections of organic photovoltaics (OPV) suitable for transmission electron microscopy (TEM) and scanning TEM (STEM) is addressed. The samples were polymer solar cells fabricated using roll-to-roll (R2R) processing methods on a flexible polyethylene terephthalate (PET) substrate. Focused ion beam (FIB) and ultramicrotomy were used to prepare the cross sections. The differences between the samples prepared by ultramicrotomy and FIB are addressed, focusing on the advantages and disadvantages of each technique. The sample prepared by ultramicrotomy yielded good resolution, enabling further studies of phase separation of P3HT:PCBM by means of energy filtered TEM (EFTEM). The sample prepared by FIB shows good structure preservation, but reduced resolution due to non-optimal thicknesses achieved after treatment. Degradation studies of samples prepared by ultramicrotomy are further discussed,
which reveal particular effects of the ISOS-L-3 aging test (85 °C, 50% R.H., 0.7 Sun) onto the sample, especially pronounced in the silver layer.

**General information**

State: Published
Number of pages: 7
Pages: 462-468
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Applied Surface Science
Volume: 389
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.951 SNIP 1.225
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.914 SNIP 1.3 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.958 SNIP 1.477 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.965 SNIP 1.488 CiteScore 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.918 SNIP 1.373 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.908 SNIP 1.402 CiteScore 2.27
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.924 SNIP 1.141
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.842 SNIP 1.023
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.899 SNIP 1.087
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.795 SNIP 0.945
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.852 SNIP 1.052
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.679 SNIP 0.946
Complementary analysis techniques applied on optimizing suspensions of yttria stabilized zirconia

Three different polymers with different functional groups and similar molecular weight were tested as dispersing agents for suspensions of yttria stabilized zirconia in ethanol: polyvinyl pyrrolidone, polyethylene imine, polyvinyl butyral/acetal. The stability of the system was assessed considering, in details, all the processing steps, including suspension de-agglomeration, slurry manipulation, quality of sintered tapes microstructure, and final layer leak tightness. Different analytical techniques were used to monitor ceramic de-agglomeration and stability as a function of time, for different types of dispersing agent and to optimize the dispersants concentration: Electrokinetic Sonic Amplitude was used to obtain zeta potential, Multiple Light Scattering for evaluating sedimentation rate, and multi-wavelength laser light scattering for measuring particle size distribution. All the results agree upon excellent performance of polyvinyl pyrrolidone and polyethylene imine as dispersing agents. The stability and dispersing power were finally utilized for preparing concentrated suspensions for tape casting and subsequently to sinter the tapes into dense ceramic pieces.
Complex hydrides as room-temperature solid electrolytes for rechargeable batteries

A central goal in current battery research is to increase the safety and energy density of Li-ion batteries. Electrolytes nowadays typically consist of lithium salts dissolved in organic solvents. Solid electrolytes could facilitate safer batteries with higher capacities, as they are compatible with Li-metal anodes, prevent Li dendrite formation, and eliminate risks associated with flammable organic solvents. Less than 10 years ago, LiBH₄ was proposed as a solid-state electrolyte. It showed a high ionic conductivity, but only at elevated temperatures. Since then a range of other complex metal hydrides has been reported to show similar characteristics. Strategies have been developed to extend the high ionic conductivity of LiBH₄ down to room temperature by partial anion substitution or nanoconfinement. The present paper reviews the recent developments in complex metal hydrides as solid electrolytes, discussing in detail LiBH₄, strategies towards for fast room-temperature ionic conductors, alternative compounds, and first explorations of implementation of these electrolytes in all-solid-state batteries.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, National Institute of Standards and Technology, Utrecht University, Tohoku University
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Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Journal: Applied Physics A
Comprehensive analysis of TEM methods for LiFePO$_4$/FePO$_4$ phase mapping: spectroscopic techniques (EFTEM, STEM-EELS) and STEM diffraction techniques (ACOM-TEM)

Transmission electron microscopy (TEM) has been used intensively in investigating battery materials, e.g. to obtain phase maps of partially (dis)charged (lithium) iron phosphate (LFP/FP), which is one of the most promising cathode material for next generation lithium ion (Li-ion) batteries. Due to the weak interaction between Li atoms and fast electrons, mapping of the Li distribution is not straightforward. In this work, we revisited the issue of TEM measurements of Li distribution maps for LFP/FP. Different TEM techniques, including spectroscopic techniques (energy filtered (EF)TEM in the energy range from low-loss to core loss) and a STEM diffraction technique (automated crystal orientation mapping (ACOM)), were applied to map the lithiation of the same location in the same sample. This enabled a direct comparison of the results. The maps obtained by all methods showed excellent agreement with each other. Because of the strong difference in the imaging mechanisms, it proves the reliability of both the spectroscopic and STEM diffraction phase mapping. A comprehensive comparison of all methods is given in terms of information content, dose level, acquisition time and signal quality. The latter three are crucial for the design of in situ experiments with beam sensitive Li-ion battery materials. Furthermore, we demonstrated the power of STEM diffraction (ACOM-STEM) providing additional crystallographic information, which can be analyzed to gain a deeper understanding of the LFP/FP interface properties such as statistical information on phase boundary orientation and misorientation between domains.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Karlsruhe Institute of Technology KIT
Authors: Mu, X. (Ekstern), Kobler, A. (Ekstern), Wang, D. (Ekstern), Chakravadhanula, V. S. K. (Ekstern), Schlabach, S. (Ekstern), Szabo, D. V. (Ekstern), Norby, P. (Intern), Kuebel, C. (Ekstern)
Number of pages: 9
Pages: 10-18
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Ultramicroscopy
Volume: 170
ISSN (Print): 0304-3991
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.82 SJR 1.915 SNIP 1.233
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.121 SNIP 1.428 CiteScore 2.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.638 SNIP 1.661 CiteScore 2.59
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.777 SNIP 1.337 CiteScore 2.66
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.867 SNIP 1.595 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Computational efficient thermo-mechanical modelling of interconnects in SOFC stacks including the effect of contact

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Mixed Conductors  
Authors: Tadesse Molla, T. (Intern), Kwok, K. (Intern), Frandsen, H. L. (Intern)  
Number of pages: 1  
Publication date: 2016  
Event: Abstract from 5th International Symposium on Energy Challenges and Mechanics, Inverness, United Kingdom.  
Main Research Area: Technical/natural sciences  
Electronic versions:  
Computational_efficient.pdf  
Source: PublicationPreSubmission  
Source-ID: 128053340  
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

**Conductivity and structure of sub-micrometric SrTiO$_3$-YSZ composites**

Sub-micrometric composites of SrTiO$_3$-YSZ (1:1 volume) and samples of SrTiO$_3$ were prepared by high temperature consolidation of precursors obtained by precipitation with NaOH. The structure development and morphology of the precursors were studied by XRD and SEM. The perovskite and fluorite phases in the composites are clearly formed at 600°C with no signs of reaction up to 1100°C; the nominally pure SrTiO$_3$ can be formed at temperatures as low as 400°C.
Composites with sub-micrometric grain sizes can be prepared successfully without reaction between the components, although a change in the cell parameter of the SrTiO$_3$ is attributed to the presence of Na. The consolidated composites were studied by impedance spectroscopy between 200 and 400°C and at a fixed temperature of 600°C with a scan in the partial pressure of oxygen. The composites did not exhibit high levels of ionic conductivity in the grain boundary nor the bulk. The conductivity of Na-free composites shows lower levels of conductivity than pure YSZ, while samples with Na showed increased conductivity. The conductivity of SrTiO$_3$ exhibited an enhancement attributed to p-type conductivity, although contributions from protons cannot be disregarded as some Na doping is present.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Fundamental Electrochemistry
Authors: Ruiz Trejo, E. (Intern), Thydén, K. T. S. (Intern), Bonanos, N. (Intern), Mogensen, M. B. (Intern)
Number of pages: 6
Pages: 82-87
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Solid State Ionics
Volume: 288
ISSN (Print): 0167-2738
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.055 SNIP 1.258 CiteScore 2.31
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.383 SNIP 1.621 CiteScore 2.96
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.459 SNIP 1.503
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.507 SNIP 1.483
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.516 SNIP 1.621
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.301 SNIP 1.392
- Web of Science (2007): Indexed yes
Conjugated Polymers for Energy Production: Finding Suitable Candidates for Low Cost Solar Cells

This dissertation is aimed at developing materials for flexible, large area, ITO-free polymer solar cells (PSCs) fully printed under ambient conditions. A large screening of conjugated polymers, both novel and well-known materials, has been carried out in order to find suitable candidates for scalable PSCs fully printed under ambient conditions [Adv. Energy Mater. 2015, 5, 1402186]. PPDTBT resulted to be the conjugated polymer with the best photovoltaic performance within the 104 synthesized macromolecules. Therefore, further studies have been done on such material. The impact of side chain position on the physical and electrical properties of PPDTBT backbone have been evaluated, finding that anchoring a branched alkoxy chain to benzene leads to PCE as high as 3.6%, a considerably high performance for flexible ITO-free PSCs (area of approx. 1 cm²) [Macromolecules 2015, 48, 3481–3492]. Direct arylation (DAr) and direct arylation polymerization (DArP) have been applied to the preparation of PPDTBT, making this polymer readily available in only 4 synthetic steps and thus easily transferable to a large scale-production setup. DArP avoids organometallic species and therefore is an appealing polymerization method for industrial production of polymers. Several DArP protocols have been employed for the synthesis of PPDTBT leading to polymers with high structural regularity and photovoltaic performances comparable with the same materials synthesized via Stille cross-coupling polymerization. The reactivity of DArP has been further studied and applied to the synthesis of fluorinated copolymers featuring thiophene, which are largely used materials for organic electronics. In particular, by moving the bromine functionality from one monomer to the other, a big impact on the reactivity has been observed. When a thiophene-based donor monomer was brominated and copolymerized with 1,2,4,5-tetrafluorobenzene, hydrodehalogenation side reactions were suppressed, leading to the synthesis of the new PTPTPf₄ defects-free copolymer [J. Polym. Sci.Part A: Polym. Chem. 2015, 53, 2598–2605].

General information
State: Published
Organisations: Functional organic materials, Department of Energy Conversion and Storage
Authors: Livi, F. (Intern), Bundgaard, E. (Intern)
Number of pages: 251
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: Conjugated_Polymers_for_Energy_Production.pdf

Relations
Projects:
Conjugated Polymers for Energy Production
Publication: Research › Ph.D. thesis – Annual report year: 2016
CO Oxidation on the Au\textsubscript{15}Cu\textsubscript{15} Cluster and the Role of Vacancies in the MgO(100) Support

A comprehensive theoretical study of a Au\textsubscript{15}Cu\textsubscript{15} cluster on MgO(100) supports and its catalytic activity for CO oxidation has been performed based on the density functional theory and microkinetic modeling. Molecular adsorption and different reaction paths based on the Langmuir–Hinshelwood (LH) and Eley–Rideal (ER) mechanisms have been explored by tuning the location of vacancies in MgO(100). The charge states of the Au\textsubscript{15}Cu\textsubscript{15} cluster are negative on all supports, defect-free, O-vacancy (F-center), and Mg-vacancy (V-center), and the effect is significantly amplified on the F-center. In each case, the O\textsubscript{2} molecule can be effectively activated upon adsorption and dissociated to 2 × O atoms easily, and the reaction modeling takes into account also the reaction paths with adsorbed O atoms. Overall, CO oxidation has lower reaction barriers on the cluster on the F-center. The microkinetic modeling analysis reveals that CO oxidation is very sensitive to the CO partial pressure, as the relatively strong CO binding leads readily to CO poisoning of the cluster surface sites and hinders CO\textsubscript{2} formation. For low CO partial pressures, the catalytic reaction takes place already at 150 K for the cluster on the F-center. The CO\textsubscript{2} production rates are much lower for the defect-free and V-center supports which display similar increased activity at elevated temperatures. In all cases, the right combination of CO and O\textsubscript{2} partial pressures is instrumental for CO\textsubscript{2} production.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Aalto University, Tampere University of Technology
Authors: Ma, L. (Ekstern), Melander, M. (Intern), Weckman, T. (Ekstern), Laasonen, K. (Ekstern), Akola, J. (Ekstern)
Pages: 26747–26758
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Volume: 120
ISSN (Print): 1932-7447
Ratings:
  - BFI (2018): BFI-level 1
  - BFI (2017): BFI-level 1
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 2.438 SNIP 1.356
  - Web of Science (2010): Indexed yes
Corrosion behavior of construction materials for ionic liquid hydrogen compressor

The corrosion behavior of various commercially available stainless steels and nickel-based alloys as possible construction materials for components which are in direct contact with one of five different ionic liquids was evaluated. The ionic liquids, namely: 1-ethyl-3-methylimidazolium triflate, 1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide, trihexyltetradecylphosphonium bis (trifluoromethylsulfonyl) imide, butyltrimethylammonium bis (trifluoromethylsulfonyl) imide, methyltrioctylammonium bis (trifluoromethylsulfonyl) imide have been identified, as performance fluids in an ionic liquid hydrogen compressor. An electrochemical cell was specially designed, and steady-state cyclic voltammetry was used to measure the corrosion resistance of the alloys in the ionic liquids at 23 °C, under atmospheric pressure.

The results showed a very high corrosion resistance and high stability for all the alloys tested. The two stainless steels, AISI 316L and AISI 347 showed higher corrosion resistance compared to AISI 321 in all the ionic liquids tested. It was observed that small addition of molybdenum, tantalum, and niobium to the alloys increased the corrosion stability in the ionic liquids studied. Hastelloy® C-276 showed the poorest corrosion resistance in all the ionic liquids tested. AISI 316L with high corrosion resistance and the lowest cost is recommended as the most attractive construction material for all the components, in an ionic liquid hydrogen compressor, which are in direct contact with ionic liquids used in this study.
Ionic liquid compressor, Hydrogen, Ionic liquids, Corrosion resistance, Polarization

DOIs:
10.1016/j.ijhydene.2016.06.221

Source: FindIt
Source-ID: 2307416474
Publication: Research - peer-review › Journal article – Annual report year: 2016

Current Constriction at Electrode/Electrolyte Interfaces in Solid Oxide Cell Electrochemical Devices Calculated Via 3D Reconstructions

Electrochemical devices such as batteries, fuel cells, electrolyzers, electrochemical reactors and electrochemical sensors are important technologies for the present and the future society. For further improvement or maturing of the various technologies it is important to understand, characterize and minimize the different losses within the devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis
Authors: Nielsen, J. (Intern), Jørgensen, P. S. (Intern), Graves, C. R. (Intern)
Publication date: 2016
Decacyclene Trianhydride at Functional Interfaces: An Ideal Electron Acceptor Material for Organic Electronics

We report the interface energetics of decacyclene trianhydride (DTA) monolayers on top of two distinct model surfaces, namely, Au(111) and Ag(111). On the latter, combined valence band photoemission and X-ray absorption measurements that access the occupied and unoccupied molecular orbitals, respectively, reveal that electron transfer from substrate to surface sets in. Density functional theory calculations confirm our experimental findings and provide an understanding not only of the photoemission and X-ray absorption spectral features of this promising organic semiconductor but also of the fingerprints associated with the interface charge transfer.

Decacyclene Trianhydride at Functional Interfaces: An Ideal Electron Acceptor Material for Organic Electronics

We report the interface energetics of decacyclene trianhydride (DTA) monolayers on top of two distinct model surfaces, namely, Au(111) and Ag(111). On the latter, combined valence band photoemission and X-ray absorption measurements that access the occupied and unoccupied molecular orbitals, respectively, reveal that electron transfer from substrate to surface sets in. Density functional theory calculations confirm our experimental findings and provide an understanding not only of the photoemission and X-ray absorption spectral features of this promising organic semiconductor but also of the fingerprints associated with the interface charge transfer.
Decoupling Strain and Ligand Effects in Ternary Nanoparticles for Improved ORR Electrocatalysis

Density functional theory is used to investigate OH adsorption on ternary Pt-Au-M (M = 3d-metal) nanoparticles in order to address their potential to improve activity for the oxygen reduction reaction (ORR) compared to pure Pt nanoparticles. The nanoparticles are investigated through a method developed for decoupling strain and ligand effects and then correlated with the extended Pt(111) surface for benchmarking. Subsurface Au has previously been shown to form a passivating layer, stabilising the nanoparticle catalysts against the harsh acidic conditions at the cathode, while the current study shows the effect of the ternary metal core allowing for tuning the catalytic activity through strain effects. Good agreement is found with experimental studies showing increased activity of Pt-Au-Fe/Ni nanoparticles, and the current study suggests that mid to late 3d-metals should also exhibit enhanced activity and stability with respect to pure Pt nanoparticles. It is suggested that the Pt-Au-M for M = Cr, Mn, Co, Cu, Zn nanoparticles are of particular interest as they exhibit an optimal interplay between strain, ligand effects and stability.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: C. Jennings, P. (Intern), Lysgaard, S. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 9
Pages: 24737-24745
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 18
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Degradation of solid oxide cells during co-electrolysis of steam and carbon dioxide at high current densities

In this work, the durability of Ni–YSZ based solid oxide cells was investigated during co-electrolysis of steam and carbon dioxide (45% H₂O + 45% CO₂ + 10% H₂) at current density of −1.5 or −2.0 A cm⁻². The cell consists of ∼300 μm Ni–YSZ support, ∼10 μm Ni–YSZ electrode, ∼10 μm YSZ electrolyte and ∼15 μm LSM–YSZ oxygen electrode. The gas conversion was 45% at −1.5 A cm⁻² and 60% at −2.0 A cm⁻², and the operating durations were up to 700 h. The detailed electrochemical analysis revealed significant increase of the ohmic resistance, oxide ion transport resistance in the
Ni–YSZ composite electrodes and the electrochemical reaction resistance at the Ni–YSZ triple-phase boundaries. The performance degradation is mainly ascribed to the microstructural change in the Ni–YSZ electrode close to the YSZ electrolyte, including the percolation loss of Ni, the contact loss between Ni and YSZ electrolyte and the decomposition of YSZ close to Ni–YSZ|YSZ interface. The electrochemical performance and the microstructure of the oxygen electrode were found to be relatively stable.

General information
State: Published
Organisations: Applied Electrochemistry, Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Tao, Y. (Intern), Ebbesen, S. D. (Intern), Mogensen, M. B. (Intern)
Number of pages: 11
Pages: 452-462
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 328
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.968 SNIP 1.726
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.597 SNIP 1.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.8 SNIP 2.224
Web of Science (2006): Indexed yes
Depth-dependent composition of sputtered ZnO:Al

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Crovetto, A. (Intern), Ottsen, T. (Ekstern), Stamate, E. (Intern), Kjær, D. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at 6th International Symposium on Transparent Conductive Materials, Chania, Greece.
Main Research Area: Technical/natural sciences
Electronic versions:
Andrea_Poster_TCM2016_final.pdf
Source: PublicationPreSubmission
Source-ID: 126934871
Publication: Research - peer-review › Poster – Annual report year: 2016

Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces
A detailed understanding of the electrochemical reduction of CO₂ into liquid fuels on rutile metal oxide surfaces is developed by using DFT calculations. We consider oxide overlayer structures on RuO₂(1 1 0) surfaces as model catalysts to elucidate the trends and limitations in the CO₂ reduction reaction (CO₂RR) based on thermodynamic analysis. We aim to specify the requirements for CO₂RR catalysts to establish adsorbate scaling relations and use these to derive activity volcanoes. Computational results show that the OH* binding free energy is a good descriptor of the thermodynamic limitations and it defines the left leg of the activity volcano for CO₂RR. HCOOH* is a key intermediate for products formed through further reduction, for example, methanediol, methanol, and methane. The surfaces that do not bind HCOOH* are selective towards formic acid (HCOOH) production, but hydrogen evolution limits their suitability. We determine the ideal binding free energy for H* and OH* to facilitate selective CO₂RR over H₂/CO evolution to be ΔG[ΔH]>0.5 eV and ΔG[ΔOH]<0.5 eV. The Re-containing overlayers considered in this work display excellent promise for selectivity, although they are active at a highly reducing potential.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Bhowmik, A. (Intern), Vegge, T. (Intern), Hansen, H. A. (Intern)
Number of pages: 15
Pages: 3230–3243
Publication date: 2016
Main Research Area: Technical/natural sciences
Design and optimization of porous ceramic supports for asymmetric ceria-based oxygen transport membranes

The microstructure, mechanical properties and gas permeability of porous supports of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-\delta}$ (CGO) were investigated as a function of sintering temperature and volume fraction of pore former for use in planar asymmetric oxygen transport membranes (OTMs). With increasing the pore former content from 11 vol% to 16 vol%, the gas permeabilities increased by a factor of 5 when support tapes were sintered to comparable densities. The improved permeabilities were due to a more favourable microstructure with larger interconnected pores at a porosity of 45% and a fracture strength of 47±2 MPa (m=7). The achieved gas permeability of 2.25×10$^{-15}$ m$^2$ for a 0.4 mm thick support will not limit the gas transport for oxygen production but in partial oxidation of methane to syngas at higher oxygen fluxes. For integration of the
CGO support layer into a flat, asymmetric CGO membrane, the sintering activity of the CGO membrane was reduced by Fe$_2$O$_3$ addition (replacing Co$_3$O$_4$ as sintering additive).

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Mixed Conductors, Forschungs Zentrum Jülich GmbH
Pages: 85-94
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Membrane Science
Volume: 513
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2 SNIP 1.771 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.433 SNIP 1.935 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.452 SNIP 2.001 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.201 SNIP 1.968 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.82 SNIP 1.726 CiteScore 4.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.821
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.638 SNIP 1.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.461 SNIP 1.805
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.474 SNIP 1.578
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.812 SNIP 2.444
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.745 SNIP 1.823
A method to determine the water vapor pressure over a corrosive substance was developed and tested with 85.5±0.4% phosphoric acid. The water vapor pressure was obtained at a range of temperatures from ∼25°C to ∼200°C using Raman spectrometry. The acid was placed in an ampoule and sealed with a reference gas (either hydrogen or methane) at a known pressure (typically ∼0.5 bar). By comparing the Raman signals from the water vapor and the references, the water pressure was determined as a function of temperature. A considerable amount of data on the vapor pressure of phosphoric acid are available in the literature, to which our results could successfully be compared. A record value of the vapor pressure, 3.40 bar, was determined at 210°C. The method required a determination of the precise Raman scattering ratios between the substance, water, and the used reference gas, hydrogen or methane. In our case the scattering ratios between water and reference ν1 Q-branches were found to be 1.20±0.03 and 0.40±0.02 for H2 and CH4, respectively.
Development of a novel rotary magnetic refrigerator

A novel rotary magnetic refrigerator was designed and built at the Federal University of Santa Catarina (UFSC). The optimized magnetic circuit is a two-pole system in a rotor-stator configuration with high flux density regions of approximately 1 T. Eight pairs of stationary regenerator beds filled with approximately 1.7 kg of gadolinium spheres (425-600 μm diameter) were placed in the magnetic gap. Two low-friction rotary valves were developed to synchronize the hydraulic and magnetic cycles. The valves were positioned at the hot end to avoid heat generation in the cold end. In this work, experimental results are presented as a function of the operating frequency, fluid flow rate, hot reservoir temperature and thermal load. The performance of the device was evaluated in terms of the coefficient of performance (COP) and overall second-law efficiency ($\eta_{2nd}$). The maximum no-load temperature span was 12 K at 1.5 Hz and 150 L h$^{-1}$, and the maximum zero-span cooling power was 150 W at 0.8 Hz and 200 L h$^{-1}$. For a thermal load of 80.4 W, at 0.8 Hz and 200 L h$^{-1}$, the device generated a temperature span of 7.1 K, with a COP of 0.54 and $\eta_{2nd}$ of 1.16%.

General information
Dry Etching

Production of large-area flat panel displays (FPDs) involves several pattern transfer and device fabrication steps that can be performed with dry etching technologies. Even though the dry etching using capacitively coupled plasma is generally used to maintain high etch uniformity, due to the need for the higher processing rates in FPDs, high-density plasma processing tools that can handle larger-area substrate uniformly are more intensively studied especially for the dry etching of polysilicon thin films. In the case of FPD processing, the current substrate size ranges from 730 × 920 mm (fourth generation) to 2,200 × 2,500 mm (eighth generation), and the substrate size is expected to increase further within a few years. This chapter aims to present relevant details on dry etching including the phenomenology, materials to be etched with the different recipes, plasma sources fulfilling the dry etching requirements, and advantages of dry etching over wet processing. Current status and future trends are also presented.

Durability Issues and Status of PBI-Based Fuel Cells

This chapter briefly reviews durability and stability issues with key materials and components for HT-PEMFCs, including the polymer membrane, the doping acid, the electrocatalyst, the catalyst support and bipolar plates. Degradation mechanisms and their dependence on fuel cell operating conditions are summarized as well. To date, lifetimes of this type of fuel cells of up to 18,000 h with degradation rates of around 5 μV/h at temperatures of 150–160 °C have been demonstrated using hydrogen and air under constant moderate load. However, the degradation rate increases by a factor 10 when the cell is exposed to start-up–shutdown or load cycling.
Ecodesign perspectives of thin-film photovoltaic technologies: A review of life cycle assessment studies

Here, we review 33 life cycle assessment (LCA) studies of thin-film photovoltaic (PV) technologies that have had a holistic coverage in their assessments and/or have included ecodesign aspects. Only five of them were found to have a comprehensive life cycle and impact coverage, and their analyses highlighted the importance of (i) including the entire life cycle of the PV system, in particular the often-omitted disposal stage, and (ii) assessing all relevant impact categories and not just climate change or energy requirements to minimise the risk of burden-shifting. Out of the 28 studies embracing ecodesign considerations in parts of the PV life cycle, the analysis of the eleven of them addressing primary energy demand during module production suggests that electricity consumption during the metal deposition processes is a top contributor and should be prioritised by PV technology developers. A similar analysis of the ten studies having included the balance of system components (BOS) in the assessments showed that these contribute significantly to most environmental impact categories. Beyond recommending that stakeholders in the PV field rely on LCA to support decision-making and to guide scientific research and technological development, we strongly advocate LCA practitioners to include the entire PV system, including the BOS, to identify ecodesign opportunities without risking potential burden-shifting across the different parts of the system and across impact categories.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Quantitative Sustainability Assessment, Department of Management Engineering
Authors: Chatzisideris, M. D. (Intern), Espinosa Martinez, N. (Intern), Laurent, A. (Intern), Krebs, F. C. (Intern)
Number of pages: 9
Pages: 2-10
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 156
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
In this paper, the energy potential of biomass from growing short rotation coppice on unused agricultural land in the Republic of Croatia is used to investigate the feasibility of Combined Heat and Power (CHP) facilities fueled by such biomass. Large areas of agricultural land that remain unused for food crops, represent significant potential for growing biomass that could be used for energy. This biomass could be used to supply power plants of up to 15MWe in accordance with heat demands of the chosen locations. The methodology for regional energy potential assessment was elaborated in previous work and is now used to investigate the conditions in which such energy facilities could be feasible. The overall potential of biomass from short rotation coppice cultivated on unused agricultural land in the scenarios with 30% of the area is up to 10PJ/year. The added value of fruit trees pruning biomass represents an incentive for the development of fruit production on such agricultural land. Sensitivity analysis was conducted for several parameters: cost of biomass, investment costs in CHP systems and combined change in biomass and technology cost.

**Economic feasibility of CHP facilities fueled by biomass from unused agriculture land: Case of Croatia**

In this paper, the energy potential of biomass from growing short rotation coppice on unused agricultural land in the Republic of Croatia is used to investigate the feasibility of Combined Heat and Power (CHP) facilities fueled by such biomass. Large areas of agricultural land that remain unused for food crops, represent significant potential for growing biomass that could be used for energy. This biomass could be used to supply power plants of up to 15MWe in accordance with heat demands of the chosen locations. The methodology for regional energy potential assessment was elaborated in previous work and is now used to investigate the conditions in which such energy facilities could be feasible. The overall potential of biomass from short rotation coppice cultivated on unused agricultural land in the scenarios with 30% of the area is up to 10PJ/year. The added value of fruit trees pruning biomass represents an incentive for the development of fruit production on such agricultural land. Sensitivity analysis was conducted for several parameters: cost of biomass, investment costs in CHP systems and combined change in biomass and technology cost.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, International Centre for Sustainable Development of Energy, Water and Environment Systems, Adria Section of the Combustion Institute, University of Zagreb

**Authors:** Pfeifer, A. (Ekstern), Dominkovic, D. F. (Intern), Ćosić, B. (Ekstern), Duić, N. (Ekstern)

**Number of pages:** 8

**Pages:** 222-229

**Publication date:** 2016
Effect of Platinum Group Metal Doping in Magnesium Diboride Wires
The effect of some platinum group metals (PGM = Rh, Pd, and Pt) on the microstructure and critical current density of Cu/Nb-sheathed MgB$_2$ wires has been studied using Mg$_{1-x}$PGM$_x$B$_2$ powders with low doping levels. It was found that Pt and Pd do not enter the MgB$_2$ lattice and have only limited influence on T$_c$. In contrast, some Rh can be substituted and induces a decrease of T$_c$. Secondary phases are formed when the solubility limit is exceeded, but they have different morphologies depending on the dopant. For some of these PGM elements, flux pinning improvements have been observed at low fields. The results are discussed in comparison with previous investigations using other transition metals for doping on the Mg site.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ecosystems Programme, University of Barcelona
Authors: Grivel, J. (Intern), Alexiou, A. (Intern), Namazkar, S. (Intern), Pitillas, A. (Ekstern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.431 SNIP 1.171 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.575 SNIP 1.27 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.364 SNIP 1.063 CiteScore 1.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.468 SNIP 1.073
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.452 SNIP 1.033
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.878 SNIP 0.987
Scopus rating (2007): SJR 0.611 SNIP 1.104
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.731 SNIP 0.935
Effect of pore formers on properties of tape cast porous sheets for electrochemical flue gas purification

Ce0.9Gd0.1O1.95 (CGO) electrolytes for electrochemical flue gas purification multilayers were fabricated by tape casting and sintering using different types, shapes and sizes of pore formers. The resulting tapes (with thickness of about 400μm) were characterized by scanning electron microscopy, gas permeability measurements, mercury porosimetry and pore orientation measurements, to investigate the role of the different pore formers on the properties after sintering at a temperature of 1250°C. Those tapes prepared from different non-spherical pore formers with comparable porosity of about 43%, showed significant differences in gas permeability which could be correlated to an increase in mean pore size and pore connectivity. The degree of pore orientation in the tape casting direction was determined by best-fit ellipse method and a modified linear intercept method and the obtained data were correlated with the corresponding gas permeability.
Research: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, Ceramic Engineering & Science
Authors: Wulff, A. C. (Intern), Molin, S. (Intern), Andersen, K. B. (Intern), Zielke, P. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

**Bibliographical note**
Sustain Abstract M-11
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
Effects of current stress and thermal storage on polymeric heterojunction P3HT:PCBM solar cell
We subjected P3HT:PCBM solar cells to electrical constant current stress and thermal storage. We employed
the impedance spectroscopy technique combined to conventional DC measurements for device characterization during all
stresses. We identified and separated different contributions affecting the open circuit voltage and short circuit current.
Several mechanisms are behind these changes during the stresses; in particular, we underlined the exciton recombination
rate and the variation of the built-in voltage.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Rizzo, A. (Ekstern), Cester, A. (Ekstern), Torto, L. (Ekstern), Barbato, M. (Ekstern), Wrachien, N. (Ekstern),
Lago, N. (Ekstern), Corazza, M. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. (Intern)
Number of pages: 6
Publication date: 2016

Effects of flow balancing on active magnetic regenerator performance
Experiments with a recently constructed rotary multi-bed active magnetic regenerator (AMR) prototype have revealed
strong impacts on the temperature span from variations in the resistances of the flow channels carrying heat transfer fluid
in and out of the regenerator beds. In this paper we show through numerical modeling how unbalanced flow in the beds
decreases the cooling power and COP for a dual bed device. Furthermore, it is shown how resistance variations in multi-
bed devices give rise to unbalanced flow in the individual beds and how this decreases cooling powers and COPs of the
machines by approximately 30% and 50%, respectively.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Nielsen, K. K. (Intern)
Number of pages: 8
Pages: 1-8
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 103
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.462 SNIP 1.828
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Effects of spark plasma sintering conditions on the anisotropic thermoelectric properties of bismuth antimony telluride

Bismuth antimony telluride (Bi$_x$Sb$_{2-x}$Te$_3$, 0.4 <x<0.6) is one of the best and most-used p-type semiconductor materials for near-room-temperature thermoelectric power generation. In this work, p-type Bi$_{0.4}$Sb$_{1.6}$Te$_3$ samples were prepared under various conditions (temperature, holding time, and ramp-rate) using spark plasma sintering (SPS). The effects of SPS conditions on the anisotropic thermoelectric properties and microstructure evolutions were systematically investigated. The change of sintering temperature showed stronger influence than other sintering parameters to the resulting thermoelectric properties. Samples sintered over the temperature range between 653 K and 773 K showed significant differences in the degrees of orientations. The change was mainly caused by grain growth and re-orientation. Despite of the anisotropy, zT value as high as 1.2 to 1.3 was achieved over the temperature range of 300 to 360 K by directly using commercial power sintered at 723 and 773 K. The sintering profiles and microstructure evolutions during SPS were illustrated and the thermoelectric properties as a function of the degrees of orientations were shown and discussed in detail.
Effects of strong cathodic polarization of the Ni-YSZ interface

Long-term strong cathodic polarization experiments of down to -2.4 V vs. $E^\circ(O_2)$ of the Ni-YSZ interface were performed at 900°C in 97% H$_2$/3% H$_2$O on model electrodes. The Ni-YSZ interface underwent extensive changes and a large affected volume with a complex microstructure and phase distribution resulted. Impedance spectroscopy shows initial decrease but later increase in the series resistance and polarization resistance during the 140-160 h of polarization, and significant inductive behavior. An intermetallic Ni-Zr phase that formed during polarization was preserved when the polarization was kept during cooling, and was identified post-mortem by transmission electron microscopy as Ni$_7$Zr$_2$. ZrO$_2$ nanoparticles were formed on the Ni-gas surface next to the Ni-YSZ-gas triple phase boundary. Explanations of the observed features are offered based on electron microscopy and impedance spectroscopy.
Effects of surface finish and mechanical training on Ni-Ti sheets for elastocaloric cooling

Elastocaloric cooling has emerged as a promising alternative to vapor compression in recent years. Although the technology has the potential to be more efficient than current technologies, there are many technical challenges that must be overcome to realize devices with high performance and acceptable durability. We study the effects of surface finish and training techniques on dog bone shaped polycrystalline samples of NiTi. The fatigue life of several samples with four different surface finishes was measured and it was shown that a smooth surface, especially at the edges, greatly improved fatigue life. The effects of training both on the structure of the materials and the thermal response to an applied strain was studied. The load profile for the first few cycles was shown to change the thermal response to strain, the structure of the material at failure while the final structure of the material was weakly influenced by the surface finish.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A P L Materials
Volume: 4
Article number: 064110
ISSN (Print): 2166-532X
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 1.889 SNIP 0.898 CiteScore 3.67
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.802 SNIP 1.055 CiteScore 3.76
Scopus rating (2014): SJR 1.525 SNIP 1.25 CiteScore 2.9
Original language: English
Shape memory effect, Surface finishing, Stress strain relations, Materials modification, Testing procedures
Electronic versions:
Effects_of_surface_finish_and_mechanical_training_on_Ni_Ti_sheets_for_elastocaloric_cooling.pdf
DOIs:
10.1063/1.4955131

Bibliographical note
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Publication: Research - peer-review › Journal article – Annual report year: 2016

Efficient modeling of metallic interconnects for thermo-mechanical simulation of SOFC stacks: homogenized behaviors and effect of contact
Currently thermo-mechanical analysis of the entire solid oxide fuel cell (SOFC) stack at operational conditions is computationally challenging if the geometry of metallic interconnects is considered explicitly. This is particularly the case when creep deformations in the interconnect are considered in addition to elasticity. In this work, this problem is addressed using homogenization, whereby the effect of the geometry is build into an effective anisotropic material law for a continuum block of material, which then represents the interconnect in the stack model. The study presents a finite element model to calculate the homogenized mechanical response of corrugated metallic interconnects at high temperatures. Thereafter, a constitutive law for the homogenized structure (effective material law) is developed. In order to properly describe the mechanical behavior of the interconnect at high temperature, deformations involving the elastic, creep as well as effect of changes in the geometry due to contact should be accounted for. The constitutive law can be applied using 3D modeling, but for simple presentation of the theory, 2D plane strain formulation is used to model the corrugated metallic interconnect. Finally, the developed constitutive law is verified by comparing its predictions for creep strain with results from the original 2D finite element model for different loading conditions. The constitutive law is found to satisfactorily describe the mechanical behavior of corrugated metallic interconnect with computational feasibility and significant speed gain.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Tadesse Molla, T. (Intern), Kwok, K. (Intern), Frandsen, H. L. (Intern)
Number of pages: 12
Pages: 6433-6444
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 41
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.142 SNIP 1.286
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.294 SNIP 1.319 CiteScore 3.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.212 SNIP 1.494 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.278 SNIP 1.467 CiteScore 3.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.515 SNIP 1.729 CiteScore 3.96
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.456 SNIP 1.837 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.589 SNIP 1.871
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.333 SNIP 1.885
Web of Science (2009): Indexed yes
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Krebs, F. C. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/-qY_3zVuA3U

Bibliographical note
Introduction
Publication: Research - peer-review › Journal article – Annual report year: 2016

Elastic Properties of the Solid Electrolyte $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO)
The oxide known as LLZO, with nominal composition $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, is a promising solid electrolyte for Li-based batteries due to its high Li ion conductivity and chemical stability with respect to lithium. Solid electrolytes may also enable the use of metallic Li anodes by serving as a physical barrier that suppresses dendrite initiation and propagation during cycling. Prior linear elasticity models of the Li electrode/solid electrolyte interface suggest that the stability of this interface is highly dependent on the elastic properties of the solid separator. For example, dendritic suppression is predicted to be enhanced as the electrolyte’s shear modulus increases. In the present study a combination of first-principles calculations, acoustic impulse excitation measurements, and nanoindentation experiments are used to determine the elastic constants and moduli for high-conductivity LLZO compositions based on Al and Ta-doping. The calculated and measured isotropic shear modulus are in good agreement, and fall within the range of 56 to 61 GPa. These values are an order of magnitude larger than for Li metal, and far exceed the minimum value (~8.5 GPa) believed to be necessary to suppress dendrite initiation. These data suggest that LLZO exhibits sufficient stiffness to warrant addition development as a solid electrolyte for Li batteries.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan, Michigan Technological University, Oak Ridge National Laboratory, RDRL-SED-C Army Research Laboratory
Elastocaloric effect of a Ni-Ti plate to be applied in a regenerator-based cooling device

The aim of this article is to analyze the elastocaloric effect of a commercial Ni-Ti plate for its application in a cooling device. In the first part, the article shows numerical results of the cooling characteristics of a regenerator-based elastocaloric cooling device with different thickness of the Ni-Ti plates based on a previously developed numerical model. It is shown that such a device (with a plate thickness of 0.1 mm) can produce a specific cooling power up to 7 kW/kg and coefficient of performance values up to 5 at the 30 K of the temperature span. In the second part of the article, a testing and analysis of the elastocaloric effect of the Ni-Ti plate using infrared thermography is shown. Prior to the elastocaloric testing, the sample was mechanically polished and subjected to 200 loading–unloading cycles at a slow strain-rate and 10,000 loading–unloading cycles at high strain-rate to stabilize its superelastic behavior and evaluate its fatigue life. When the functional and structural stability was reached and relatively good fatigue resistance was proven, the elastocaloric effect of the sample was studied with an infrared camera as a function of strain-rate and applied strain. It is shown that the adiabatic conditions are well approximated at strain-rates above 0.1 s⁻¹. The largest adiabatic temperature change of 14 K during loading and 12.5 K during unloading were measured at the applied strain of 4.2% (at a strain-rate of 0.33 s⁻¹). The homogeneity of the elastocaloric effect and the temperature irreversibilities during unloading are presented and discussed. It can be concluded that thin Ni-Ti plates with suitable austenitic finish temperature are good candidates to be applied in a proof-of-concept regenerator-based cooling device.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Tusek, J. (Intern), Engelbrecht, K. (Intern), Pryds, N. (Intern)
Number of pages: 11
Pages: 489-499
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Science and Technology for the Built Environment
Volume: 22
Issue number: 5
ISSN (Print): 2374-4731
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.01
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.514 SNIP 0.731
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.561 SNIP 0.891
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.544 SNIP 1.104
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Electric field control of the γ-Al₂O₃/SrTiO₃ interface conductivity at room temperature

Controlling interfaces using electric fields is at the heart of modern electronics. The discovery of the conducting interface between the two insulating oxides LaAlO₃ (LAO) and SrTiO₃ (STO) has led to a number of interesting electric field-dependent phenomena. Recently, it was shown that replacing LAO with a spinel γ-Al₂O₃ (GAO) allows a good pseudo-epitaxial film growth and high electron mobility at low temperatures. Here, we show that the GAO/STO interface resistance, similar to LAO/STO, can be tuned by orders of magnitude at room temperature using the electric field of a backgate. The resistance change is non-volatile, bipolar, and can be tuned continuously rather than being a simple on/off switch. Exposure to light significantly changes the capabilities to tune the interface resistance. High- and low-resistive states are obtained by annihilation and creation, respectively, of free n-type carriers, and we speculate that electromigration of oxygen vacancies is the origin of the tunability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Copenhagen
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 109
Issue number: 2
Article number: 021602
ISSN (Print): 0003-6951
Ratings:

- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 2.67 SJR 1.132 SNIP 0.996
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.799 SNIP 1.462 CiteScore 3.25
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 2.149 SNIP 1.652 CiteScore 3.77
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 2.554 SNIP 1.754 CiteScore 3.76
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 2.805 SNIP 1.94 CiteScore 4.04
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.926 SNIP 1.789
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 2.857 SNIP 1.848
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 2.934 SNIP 1.83
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 3.039 SNIP 1.913
- Web of Science (2007): Indexed yes
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 3.709 SNIP 2.382
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 3.904 SNIP 2.38
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 3.765 SNIP 2.27
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 3.917 SNIP 2.365
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 4.111 SNIP 2.212
- Web of Science (2001): Indexed yes
- Scopus rating (2000): SJR 4.277 SNIP 2.013
- Web of Science (2000): Indexed yes
- Scopus rating (1999): SJR 4.35 SNIP 2.11

Original language: English

Magnetization reversals, Electric fields, Vacancies, Electrical resistivity, Heterojunctions

DOIs:
Electrochemical Characterization of PEMECs Operating at Various Current Densities

This conference contribution touches upon electrochemical characterization of operating polymer electrolyte membrane electrolysis cells (PEMECs) by the application of electrochemical impedance spectroscopy (EIS). Analysis of differences in impedance spectra (ADIS) (Jensen et al., 2007) can be applied to gain insight into the relative magnitudes of resistance contributions from the two electrodes, the electrolyte and of mass transfer limitations and can help identifying the time scale of the respective processes. The gained knowledge may facilitate further development of the PEMECs.

General information
State: Published
Authors: Elsøe, K. (Intern), G.-Madsen, L. (Ekstern), Scherer, G. G. (Ekstern), Hjelm, J. (Intern), Mogensen, M. B. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Issue number: 38
Article number: 2408
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org/content/MA2016-02/38/2408.abstract?sid=f6e5ab15-e4a2-45ba-82f8-17751791c37
Source: FindIt
Source-ID: 2344805999
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Electrochemical Impedance Spectroscopy on Industrially-Relevant Solid Oxide Electrolyzer Cell Stacks: A Powerful Tool for in-Situ Investigations of Degradation Mechanisms

In the current efforts of moving energy production to renewable sources, wind and solar energy are widely considered as the key technologies to cover our growing demands. However, the fluctuating nature of these sources requires a flexible energy system and storage technologies to ensure that energy services can be covered in a stable and affordable manner. One promising solution is the synthetic fuel production by solid oxide electrolyzers. Electricity can be stored in a power-to-gas process during times of excess electricity production and then further converted to liquid fuels for e.g. transportation, or at high demands converted back to electricity by either conventional power plants or fuel cells.

One of today’s biggest hurdles for a successful commercialization of solid oxide electrolyzers is the stack’s lifetime with current industry targets in the order of five to ten years. To identify and quantify the different degradation mechanisms sensitive in-situ analysis tools are needed. On single cell level, electrochemical impedance spectroscopy (EIS) is a well-established diagnostics tool. On stack level EIS has been shown to be more difficult because of geometrical restrictions of the stack design and significantly lower resistances due to the larger active cell area. Nevertheless, it is becoming a more and more important technique for stack diagnostics.

Here we present impedance spectroscopy results of two solid oxide stacks provided by Haldor Topsoe A/S. The first stack was a 14-cell stack (Delta design) specifically optimized for EIS measurements, while the other stack was an 8-cell stack (TSP-1 design), where impedance measurements were carried out without major modifications to the stack. The individual cell voltages were monitored simultaneously by EIS during up to 2000 hours in electrolysis within the ForskEL project 2015-1-12276 “Towards Solid Oxide Electrolysis Plants in 2020”, funded by Danish Energet.dk. The analysis provides valuable insight into the degradation processes which could not have been obtained by current-voltage-data alone.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry, Haldor Topsoe AS
Authors: Zielke, P. (Intern), Høgh, J. V. T. (Intern), Chen, M. (Intern), Kiebach, W. (Intern), Künkas, R. (Ekstern), Blennow, P. (Ekstern), Hjelm, J. (Intern), Hendriksen, P. V. (Intern)
Electrochemically Scavenging the Silica Impurities at the Ni-YSZ Triple Phase Boundary of Solid Oxide Cells

Silica impurity originated from the sealing or raw materials of the solid oxide cells (SOCs) accumulating at the Ni-YSZ triple phase boundaries (TPBs) is known as one major reason for electrode passivation. Here we report nanosilica precipitates inside Ni grains instead of blocking the TPBs when operating the SOCs at vertical $|i| \geq 1.5$ A cm$^{-2}$ for electrolysis of H$_2$O/CO$_2$. An electrochemical scavenging mechanism was proposed to explain this unique behavior: the removal of silica proceeded through the reduction of the silica to Si under strong cathodic polarization, followed by bulk diffusion of Si into Ni and reoxidation of Si in the Ni grain.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, University of Oslo, West Virginia University
Authors: Tao, Y. (Ekstern), Shao, J. (Intern), Cheng, S. (Ekstern)
Number of pages: 5
Pages: 17023-17027
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: A C S Applied Materials and Interfaces
Volume: 8
Issue number: 27
ISSN (Print): 1944-8244
Ratings:
  BFI (2018): BFI-level 2
  BFI (2017): BFI-level 1
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 1
  Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
Electrochemical Reduction of NO2

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Shenzhen University
Authors: Shao, J. (Ekstern), Holtappels, P. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 1
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-01
Article number: 1373
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
Electrochemical_Reduction_of_NO2.pdf
Links:
http://ma.ecsdl.org/content/MA2016-01/28/1373.abstract?sid=abc96dbb-3b67-49ec-9588-ac0ca9a0cc45
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Electrochemical removal of NOx using solid oxide cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Kammer Hansen, K. (Intern), Traulsen, M. L. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Electrochemistry 2016, Goslar, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
Electrochemical removal
Publication: Research › Conference abstract for conference – Annual report year: 2016

Electrochemical Studies of Corrosion in Liquid Electrolytes for Energy Conversion Applications at Elevated Temperatures
Stainless steels (AISI 316, 321 and 347), high-nickel alloys (Hasteloy®C-276 and Inconel®625), tantalum, nickel, titanium, tungsten, molybdenum, niobium, platinum, and gold were tested for corrosion resistance in molten KH2PO4 (or KH2PO4-K2H2P2O7) as a promising electrolyte for the intermediate-temperature (200–400°C) water electrolysis. Pt, Ta, Nb, Ti, Inconel®625, and Ni demonstrated high corrosion resistance. Au and the rest of the tested materials were not corrosion resistant. It means that Ni, Ti and Inconel®625 may be used as relatively cheap construction materials for the intermediate-temperature water electrolyzer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Nikiforov, A. V. (Intern), Petrushina, I. (Intern), Bjerrum, N. J. (Intern)
Electrodeposition of metallic 3D surface-profiles for superconductor tapes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Department of Physics
Authors: Wulff, A. C. (Intern), Jørgensen, P. S. (Intern), Nielsen, P. H. (Intern), Hansen, J. O. B. (Ekstern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Published: September 7, 2016 under CC BY 3.0 license. © The Author(s).
Source: PublicationPreSubmission
Source-ID: 127149620
Publication: Research - peer-review › Book chapter – Annual report year: 2016

Electronic Structure of Low-Dimensional Carbon Π-Systems

X-ray absorption spectroscopy (XAS) is combined with density functional theory (DFT) to determine the orbitals of one- and two-dimensional carbon Π-systems (lycopene, beta-carotene, retinal, retinol, retinoic acid, coronene, triphenylene). Considerable fine structure is observed for the transition from the C is level to the lowest unoccupied molecular orbital (LUMO) and explained by DFT. The wave functions of the one-dimensional chain molecules display the node structure of a vibrating string. The XAS transition energy is decomposed into contributions from the C is core level, the Π* final state, and the electron hole interaction. For the latter, we develop a simple model that accurately represents a full Delta-self-consistent field (ΔSCF) calculation. The distortion of the LUMO because of its interaction with the C is hole is investigated. These results illustrate the electronic states of prototypical Π-bonded carbon structures with low-dimensional character, such as those used in molecular complexes for solar cells, confined graphene structures, and molecular wires.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Wisconsin-Madison, Lawrence Berkeley National Laboratory, Max Planck Institute for the Structure and Dynamics of Matter
Authors: García Lastra, J. M. (Intern), Boukahil, I. (Ekstern), Qiao, R. (Ekstern), Rubio, A. (Ekstern), Himpsel, F. J. (Ekstern)
Number of pages: 7
Pages: 12362-12368
Publication date: 2016
Main Research Area: Technical/natural sciences
Electron microscopy investigations of changes in morphology and conductivity of LiFePO4/C electrodes

In this work we study the structural degradation of a laboratory Li-ion battery LiFePO4/Carbon Black (LFP/CB) cathode by various electron microscopy techniques including low kV Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) 3D tomography. Several changes are observed in FIB/SEM images of fresh and degraded cathodes, including cracks in the LFP particles, secondary disconnected particles, and agglomeration of CB. Low voltage (1 kV) SEM images show that the CB agglomerates have a different brightness than the fresh CB, due to charging effects. This suggests that the electronic conductivity of the CB agglomerates is low compared to that of the fresh CB particles. HRTEM analysis shows that fresh CB particles are quasi crystalline, whereas the LFP/CB interface in the degraded electrode shows amorphous carbon surrounding the LFP particles. The presence of the amorphous carbon is known to impede the electronic conductivity and thereby decreasing percolation in the cathode and reducing the electrode capacity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Atomic scale modelling and materials, Northwestern University
Number of pages: 11
Pages: 259-269
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 307
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Electro-Oxidative Conversion and Process Intensification of Biomass derived 5-Hydroxymethylfurfural into 2,5-furandicarboxylic acid

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Joya, K. S. (Intern), Chatzichristodoulou, C. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
Research › Conference abstract for conference – Annual report year: 2016

Electroreduction of N2 to ammonia at ambient conditions on mononitrides of Zr, Nb, Cr, and V – A DFT guide for experiments

A rapid and facile reduction of nitrogen to achieve a sustainable and energy efficient production of ammonia is critical to its use as a hydrogen storage medium, chemical feedstock and especially for manufacturing inorganic fertilizers. For a decentralization of catalytic ammonia production, small-scale N2 reduction devices are required that are equipped with the most stable, selective and active catalysts that operate at low temperature and ambient pressure. Here, we report the development of new and cost-efficient catalysts, transition metal nitrides, which enable electrochemical reduction of molecular nitrogen to ammonia in aqueous media at ambient conditions with only a low applied bias. The most promising catalysts are VN, ZnN, NbN and CrN, which are identified among a range of transition metal nitride surfaces through a comprehensive density functional theory based analysis. All four nitrides are found to be more active towards nitrogen reduction than towards the competing hydrogen evolution reaction, in contrast to pure metal catalysts, which largely evolve hydrogen. Furthermore, their stability against poisoning and possible decomposition under operating conditions is also studied. Particular single-crystal surfaces are needed for ZrN, NbN and CrN because polycrystalline surfaces may result in decomposition of the whole catalyst. Polycrystalline surfaces of VN may, however, be used since the rocksalt (100) facet is predicted to produce ammonia via a Mars-van Krevelen mechanism with only a ~0.5 V overpotential, thereby avoiding decomposition. We suggest that this is a promising step towards the development of a method for synthesizing ammonia cheaply, to prepare high-value-added nitrogenous compounds directly from air, water and electricity at ambient conditions. An additional benefit to the present analysis is that the method used in this work may be applicable to other
aqueous phase catalytic reactions, where a Mars-van Krevelen mechanism is operative and product selectivity and activity are key catalytic criteria.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Iceland, University of Otago  
**Authors:** Abghoui, Y. (Ekstern), Garden, A. L. (Ekstern), Howalt, J. G. (Intern), Vegge, T. (Intern), Skúlason, E. (Ekstern)  
**Pages:** 635–646  
**Publication date:** 2016  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** A C S Catalysis  
**Volume:** 6  
**ISSN (Print):** 2155-5435  
**Ratings:**  
- BFI (2018): BFI-level 1  
- BFI (2017): BFI-level 1  
- Web of Science (2017): Indexed yes  
- BFI (2016): BFI-level 1  
- Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071  
- Web of Science (2016): Indexed yes  
- BFI (2015): BFI-level 1  
- Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88  
- Web of Science (2015): Indexed yes  
- BFI (2014): BFI-level 1  
- Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74  
- Web of Science (2014): Indexed yes  
- BFI (2013): BFI-level 1  
- Scopus rating (2013): SJR 3.271 SNIP 1.859 CiteScore 7.41  
- ISI indexed (2013): ISI indexed yes  
- Web of Science (2013): Indexed yes  
- Scopus rating (2012): SJR 2.684 SNIP 1.61 CiteScore 5.19  
- ISI indexed (2012): ISI indexed no  
- Web of Science (2012): Indexed yes  
- ISI indexed (2011): ISI indexed no  
**Original language:** English  
**DOIs:**  
10.1021/acscatal.5b01918

Elucidating Batch-to-Batch Variation Caused by Homocoupled Side Products in Solution-Processable Organic Solar Cells

Conjugated polymers and small molecules based on alternating electron-donating (D) and electron-accepting (A) building blocks have led to state-of-the-art organic solar cell materials governing efficiencies beyond 10%. Unfortunately, the connection of D and A building blocks via cross-coupling reactions does not always proceed as planned, which can result in the generation of side products containing D-D or A-A homocoupling motifs.Previous studies have reported a reduced performance in polymer and small molecule solar cells when such defect structures are present. A general consensus on the impact of homocouplings on device performance is, however, still lacking as is a profound understanding of the underlying causes of the device deterioration. For differentiating the combined effect of molecular weight and homocouplings in polymer solar cells, a systematic study on a small molecule system (DTS(FBBTh2)2) is presented. The impact of homocouplings on nanomorphology, thermal, and electro-optical properties is investigated. It is demonstrated that small quantities of homocouplings (
Enhanced proton conductivity of niobium phosphates by interfacing crystal grains with an amorphous functional phase

Niobium phosphate is an interesting proton conductor operational in the intermediate temperature range. In the present work two forms of phosphates were prepared: an amorphous one with high specific area and a crystalline one with low specific surface area. Both phosphates exhibited very low proton conductivities. An activation process was developed to convert the phosphates into crystal grains with a phosphorus rich amorphous phase along the grain boundaries. As a result, the obtained niobium phosphates showed considerably enhanced and stable proton conductivities. The activation effect was prominent when the high surface area amorphous phosphate was used as the precursor. At 250 °C thus obtained niobium phosphate showed a high and stable conductivity of 0.03 S cm⁻¹ under dry atmosphere and of 0.06 S cm⁻¹ at a water partial pressure of 0.12 atm.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, China University of Geosciences
Authors: Huang, Y. (Ekstern), Yu, L. (Ekstern), Li, H. (Ekstern), Wang, C. (Ekstern), Li, Q. (Intern), Shuai, Q. (Ekstern)
Number of pages: 5
Pages: 54-58
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 294
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.055 SNIP 1.258 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.383 SNIP 1.621 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.459 SNIP 1.503
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.507 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.516 SNIP 1.621
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.301 SNIP 1.392
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.235 SNIP 1.543
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.088 SNIP 1.431
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.182 SNIP 1.556
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.456 SNIP 1.401
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.376 SNIP 1.35
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.123 SNIP 1.216
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.997 SNIP 1.321
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.107 SNIP 1.26
Original language: English
DOIs:
10.1016/j.ssi.2016.06.018
Source: FindIt
Source-ID: 2306640019
Publication: Research - peer-review › Journal article – Annual report year: 2016
Epoxy-bonded La(Fe,mn,si)$_{13}$H$_x$ As A Multi Layered Active Magnetic Regenerator

The high magnetocaloric effect and tunability of the Curie temperature over a broad range makes La(Fe,Mn,Si)$_{13}$H$_x$ a promising magnetocaloric material for applications. Due to a volume change across the transition and the brittleness of the material as well as erosion due to fluid flow, the particles of the material may break apart during operation. In this context, we studied epoxy-bonded La(Fe,Mn,Si)$_{13}$H$_x$ regenerators, in a small versatile active magnetic regeneration (AMR) test device with a 1.1 T permanent magnet source. The magnetocaloric material was in the form of packed irregular particles (250-500 µm), which were mechanically held in place by an epoxy matrix connecting the particles, improving the mechanical integrity, while allowing a continuous porosity for the fluid flow. Water with 2 wt% ENTEK FNE as anti-corrosion additive was used as the heat transfer fluid for the epoxy-bonded regenerators. A series of AMRs was evaluated by varying the epoxy content in the range 1-4 wt%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Vacuumschmelze GmbH & Co. KG
Authors: Neves Bez, H. (Intern), Navickaitė, K. (Intern), Lei, T. (Intern), Engelbrecht, K. (Intern), Barcza, A. (Ekstern), Bahl, C. (Intern)
Number of pages: 6
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 7th International Conference on Magnetic Refrigeration at Room Temperature
Publisher: IIF-IIR
Main Research Area: Technical/natural sciences
Magnetocaloric, Refrigeration, Epoxy-bonded, Layered regenerator, AMR

Evidence for lattice-polarization-enhanced field effects at the SrTiO$_3$-based heterointerface

Electrostatic gating provides a powerful approach to tune the conductivity of the two-dimensionalelectron liquid between two insulating oxides. For the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface, such gating effect could be further enhanced by a strong lattice polarization of STO caused by simultaneous application of gate field and illumination light. Herein, by monitoring the discharging process uponremoving the gate field, we give firm evidence for the occurrence of this lattice polarization at the amorphous-LaAlO$_3$/SrTiO$_3$ interface. Moreover, we find that the lattice polarization is accompanied with a large expansion of the out-of-plane lattice of STO. Photo excitation affects the polarization process by accelerating the field-induced lattice expansion. The present work demonstrates the great potential of combined stimuli in exploring emergent phenomenon at complex oxide interfaces.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences
Authors: Li, Y. (Ekstern), R. Zhang, H. (Ekstern), Lei, Y. (Ekstern), Chen, Y. (Intern), Pryds, N. (Intern), Shen, B. (Ekstern), Sun, J. (Ekstern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 22418
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
Web of Science (2016): Indexed yes
Evidence of weak superconductivity at the room-temperature grown LaAlO_3/SrTiO_3 interface

The two-dimensional electron gas at the crystalline LaAlO_3/SrTiO_3 (c-LAO/STO) interface has sparked large interest due to its exotic properties, including an intriguing gate-tunable superconducting phase. While there is growing evidence of pronounced spatial inhomogeneity in the conductivity at STO-based interfaces, the consequences for superconductivity remain largely unknown. We study interfaces based on amorphous LAO top layers grown at room temperature (a-LAO/STO) and demonstrate a superconducting phase similar to c-LAO/STO, however, with a gate-tunable critical temperature of 460 mK. The dependence of the superconducting critical current on temperature, magnetic field, and back-gate-controlled doping is found to be consistently described by a model of a random array of Josephson-coupled superconducting domains.
Evolution of the electrochemical interface in high-temperature fuel cells and electrolyser

The critical region determining the performance and lifetime of solid oxide electrochemical systems is normally at the electrode side of the electrode/electrolyte interface. Typically this electrochemically active region only extends a few micrometres and for best performance involves intricate structures and nanocomposites. Much of the most exciting recent research involves understanding processes occurring at this interface and in developing new means of controlling the
structure at this interface on the nanoscale. Here we consider in detail the diverse range of materials architectures that may be involved, describe the evolution of these interface structures and finally explore the new chemistries that allow control and manipulation of these architectures to optimize both performance and durability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, University of St Andrews
Number of pages: 13
Publication date: 2016
Main Research Area: Technical/natural sciences

Exceptional durability enhancement of PA/PBI based polymer electrolyte membrane fuel cells for high temperature operation at 200°C
The incorporation of phosphotungstic acid functionalized mesoporous silica in phosphoric acid doped polybenzimidazole (PA/PBI) substantially enhances the durability of PA/PBI based polymer electrolyte membrane fuel cells for high temperature operation at 200°C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Curtin University of Technology (Curtin University), Deakin University, University of Queensland
Number of pages: 6
Pages: 4019-4024
Publication date: 2016
Main Research Area: Technical/natural sciences
Experimental and theoretical investigation of Cr$_{1-x}$Sc$_x$N solid solutions for thermoelectrics

The ScN- and CrN-based transition-metal nitrides have recently emerged as a novel and unexpected class of materials for thermoelectrics. These materials constitute well-defined model systems for investigating mixing thermodynamics, phase stability, and band structure aiming for property tailoring. Here, we demonstrate an approach to tailor their thermoelectric properties by solid solutions. The trends in mixing thermodynamics and densities-of-states (DOS) of rocksalt-Cr$_1$-xSc$_x$N solid solutions (0 ≤ x ≤ 1) are investigated by first-principles calculations, and Cr$_1$-xSc$_x$N thin films are synthesized by magnetron sputtering. Pure CrN exhibits a high power factor, 1.7 × 10$^{-3}$ W m$^{-1}$ K$^{-2}$ at 720 K, enabled by a high electron concentration thermally activated from N vacancies. Disordered rocksalt-Cr$_1$-xSc$_x$N solid solutions are thermodynamically stable, and calculated DOS suggest the possibility for power-factor improvement by Sc3d orbital delocalization on Cr3d electrons giving decreasing electrical resistivity, while localized Cr3d orbitals with a large DOS slope may yield an improved Seebeck coefficient. Sc-rich solid solutions show a large improvement in power factor compared to pure ScN, and all films have power factors above that expected from the rule-of-mixture. These results corroborate the theoretical predictions and enable tailoring and understanding of structure-transport-property correlations of Cr$_1$-xSc$_x$N.
Experimental performance evaluation of sintered Gd spheres packed beds

Research in magnetic refrigeration heavily relies on the use of packed spheres in regenerators, however little investigation to verify that such non-monolithic arrangements guarantee a sufficiently constrained structure has yet been performed. This work presents a preliminary comparison of the performance of AMRs consisting of Gd spheres with diameters ranging from 450-550 microns partially sintered by Spark Plasma Sintering (SPS) to similar spheres, sorted in the same size range and from the same batch, but merely packed. Pressure drop is compared at uniform temperature and at a range of heat rejection temperatures and temperature spans. Performance is compared in terms of temperature span at a range of heat rejection temperatures (295-308 K) and 0 and 10 W cooling loads. Results show a moderate increase of pressure drop with the sintered spheres, while temperature spans were consistently 2.5-5 K smaller. These results are coherent with previously presented results [1].
Exploring product development possibilities and alternative uses of PV solar cells in Ghana

General information
State: Published
Organisations: Department of Management Engineering, UNEP DTU Partnership, Department of Energy Conversion and Storage, Secretariat, IT, Ashesi University, Kwame Nkrumah University of Science and Technology
Authors: Adomdza, G. K. (Ekstern), McBagonluri, F. (Ekstern), Kemausour, F. (Ekstern), Nygaard, I. (Intern), Hansen, U. E. (Intern), Lauritzen, H. (Intern)
Publication date: 2016

Exploring the efficiency potential for an active magnetic regenerator

A novel rotary state of the art active magnetic regenerator refrigeration prototype was used in an experimental investigation with special focus on efficiency. Based on an applied cooling load, measured shaft power, and pumping power applied to the active magnetic regenerator, a maximum second-law efficiency of 18% was obtained at a cooling load of 81.5 W, resulting in a temperature span of 15.5 K and a coefficient of performance of 3.6. A loss analysis is given, based on measured pumping power and shaft power together with theoretically estimated regenerator pressure drop. It is shown that, especially for the pressure drop, significant improvements can be made to the machine. However, a large part of the losses may be attributed to regenerator irreversibilities. Considering these unchanged, an estimated upper limit to the second-law efficiency of 30% is given by eliminating parasitic losses and replacing the packed spheres with a theoretical parallel plate regenerator. Furthermore, significant potential efficiency improvements through optimized regenerator geometries are estimated and discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Haffenden Bahl, C. R. (Ekstern), Bjørk, R. (Intern)
Number of pages: 7
Around 9%, with sputtering. Did you manage to get good quality CZTS? We cannot evaluate the performance of our annealing + device processing we reached a PLD record efficiency of 5.2%. The world record efficiency for this material is a 2.6% conversion efficiency. With the absorber layer produced with our PLD setup followed by a well established PLD step to the final device efficiency. What is your best solar cells? With our own in-house device fabrication we reached temperature and then annealed in a furnace with some sulfur powder aside. The annealing step is as important as the How to do it? I suggest to do PLD on a single sintered target (2CuS:ZnS:SnS) .The films are deposited at room see how material transfer in PLD, which is generally believed to be stoichiometric, can be very much non-stoichiometric. to deposit a thin film CZTS absorber layer with Pulsed Laser Deposition with the desired composition. In addition, you will absorber layer alone. The only meaningful information comes from the full solar cell operation, but at this stage everything "good" or "bad" CZTS only using conventional techniques (Raman, SEM, X-ray diffraction, photoluminescence..) on the absorber layer alone. The only meaningful information comes from the full solar cell operation, but at this stage everything is coupled together behind the Quantum Efficiency (QE) curve. What do I learn by reading this thesis? You will learn how to deposit a thin film CZTS absorber layer with Pulsed Laser Deposition with the desired composition. In addition, you will see how material transfer in PLD, which is generally believed to be stoichiometric, can be very much non-stoichiometric. How to do it? I suggest to do PLD on a single sintered target (2CuS:ZnS:SnS). The films are deposited at room temperature and then annealed in a furnace with some sulfur powder aside. The annealing step is as important as the PLD step to the final device efficiency. What is your best solar cells? With our own in-house device fabrication we reached a 2.6% conversion efficiency. With the absorber layer produced with our PLD setup followed by a well established annealing + device processing we reached a PLD record efficiency of 5.2%. The world record efficiency for this material is around 9%, with sputtering. Did you manage to get good quality CZTS? We cannot evaluate the performance of our
annealing step. We can only demonstrate that the precursors made with PLD can be used for producing state-of-the-art solar cells. Is there anything left to do? Oh yes! Exploring the non-equilibrium properties of PLD for the production of CZTS films. This may enable one to deposit crystalline CZTS at lower substrate temperature, with no requirement for an annealing step afterwards. Preliminary results do not seem too encouraging. The main obstacle to this approach may be that droplets do not have enough thermal energy to dissociate and merge in the absorber layer. Any further suggestions? Learn by doing. Results from other group are more-often-than-not system dependent. Select your references very carefully. If the paper doesn't come from a group that has ever reported making solar cells, there is almost no point in reading it (and they are the vast majority).

**Vox auctoritatis:**

"[...] the thickness of annealed films was 1.7μm for CZTSSe, and 0.9μm for CZTS (significant cracks will develop for a thicker CZTS lm).", from a foot-note in IBM's [34], Dec. 2015. And I really wish they had written this before.

"[...] even rather detailed materials characterization was not able to resolve the particular chemical products that led to the large differences in device performance. The devices in this study varied from 0.3% to 7.9% efficient, but no strong differences were observed by Raman, SEM, or EDS mapping at the surfaces and back contacts. This means that the causes of the electrical differences are on a smaller scale than the resolution of these techniques and could be, for example, very finely distributed secondary phases, changes in grain boundaries, or of course, point defects.", from a paper by J. Scragg dated 2013 [29]. Which basically says that if you do not make a solar cell, you do not understand much about this material.

"of course you can talk about XRD, at some point you've got to write something to finish your phD, but people mostly care about optical and electronic properties of this material, and of course, the efficiency of the solar cell above all". Private discussion with S. Siebentritt.

"[...] you just need to have the right composition in your precursors and the annealing pretty much does the job". Private discussion with T. Teodorov, from IBM's lab.

"[...] reproducibility of the results is an issue. Reproducibility of our best solar cells is below 30%". Private discussion with S. Tajima, from Toyota's lab.
Flexible ITO-free organic solar cells applying aqueous solution-processed V2O5 hole transport layer: An outdoor stability study

Solution processable semiconductor oxides have opened a new paradigm for the enhancement of the lifetime of thin film solar cells. Their fabrication by low-cost and environmentally friendly solution-processable methods makes them ideal...
Barrier (hole and electron) transport layers. In this work, we fabricate flexible ITO-free organic solar cells (OPV) by printing methods applying an aqueous solution-processed V2O5 as the hole transport layer (HTL) and compared them to devices applying PEDOT:PSS. The transparent conducting electrode was PET/Ag/PEDOT/ZnO, and the OPV configuration was PET/Ag/PEDOT/ZnO/P3HT:PC60BM/HTL/Ag. Outdoor stability analyses carried out for more than 900 h revealed higher stability for devices fabricated with the aqueous solution-processed V2O5.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Universidade Federal do Ceará, Universidade Autónoma de Barcelona, Universidade Estadual do Centro Oeste
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: A P L Materials
Volume: 4
Article number: 026104
Ratings:
ISI indexed (2013): ISI indexed no
Original language: English
Electronic versions:
Flexible_ITO_free.pdf
DOIs:
10.1063/1.4942638

**Bibliographical note**
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Source: PublicationPreSubmission
Source-ID: 121913963
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Flow Synthesis of Silver Nanowires for Semitransparent Solar Cell Electrodes: A Life Cycle Perspective**
Silver nanowires (AgNWs) were prepared on a 5g scale using either the well-known batch synthesis following the polyol method or a new flow synthesis method. The AgNWs were employed as semitransparent electrode materials in organic photovoltaics and compared to traditional printed silver electrodes based on micron sized silver flakes using life cycle analysis and environmental impact analysis methods. The life cycle analysis of AgNWs confirms that they provide an avenue to low-impact semitransparent electrodes. We find that the benefit of AgNWs in terms of embodied energy is less pronounced than generally assumed but that the toxicological and environmental benefits are significant.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Espinosa Martínez, N. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 8
Pages: 893–899
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: ChemSusChem (Print)
Volume: 9
Issue number: 8
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.385 SNIP 1.276
Flow synthesis - the answer to reproducible high-performance conjugated polymers on the scale that R2R processing demands

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Helgesen, M. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/S1KSjEnRJgM

Bibliographical note
Invited talk

Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2016
Formation of copper tin sulfide films by pulsed laser deposition at 248 and 355 nm
The influence of the laser wavelength on the deposition of copper tin sulfide (CTS) and SnS-rich CTS with a 248-nm KrF excimer laser (pulse length τ = 20 ns) and a 355-nm frequency-tripled Nd:YAG laser (τ = 6 ns) was investigated. A comparative study of the two UV wavelengths shows that the CTS film growth rate per pulse was three to four times lower with the 248-nm laser than the 355-nm laser. SnS-rich CTS is more efficiently ablated than pure CTS. Films deposited at high fluence have submicron and micrometer size droplets, and the size and area density of the droplets do not vary significantly from 248 to 355 nm deposition. Irradiation at low fluence resulted in a non-stoichiometric material transfer with significant Cu deficiency in the as-deposited films. We discuss the transition from a non-stoichiometric material transfer at low fluence to a nearly stoichiometric ablation at high fluence based on a transition from a dominant evaporation regime to an ablation regime.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnoloy, Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Authors: Ettlinger, R. B. (Intern), Crovetto, A. (Intern), Canulescu, S. (Intern), Cazzaniga, A. C. (Intern), Ravnkilde, L. (Ekster), Youngman, T. H. (Intern), Hansen, O. (Intern), Pryds, N. (Intern), Schou, J. (Intern)
Number of pages: 10
Pages: 1-10
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Physics A
Volume: 122
Issue number: 4
ISSN (Print): 0947-8396
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.52 SJR 0.101 SNIP 0.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.1 SNIP 0 CiteScore 1.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.113 SNIP 0.002 CiteScore 1.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.1 SNIP 0 CiteScore 1.75
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.1 SNIP 0 CiteScore 1.71
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.866 SNIP 1.129 CiteScore 1.77
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.064 SNIP 1.029
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
From a magnet to a heat pump

The magnetocaloric effect (MCE) is the thermal response of a magnetic material to an applied magnetic field. Magnetic cooling is a promising alternative to conventional vapor compression technology in near room temperature applications and has experienced significant developments over the last five years. Although further improvements are necessary before the technology can be commercialized. Researchers were mainly focused on the development of materials and optimization of a flow system in order to increase the efficiency of magnetic heat pumps. The project, presented in this paper, is devoted to the improvement of heat pump and cooling technologies through simple tests of prospective regenerator designs. A brief literature review and expected results are presented in the paper. It is mainly focused on MCE technologies and provides a brief introduction to the magnetic cooling as an alternative for conventional vapor compression technology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Pages: 73-79
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Sustainable Architecture and Civil Engineering
Volume: 14
Issue number: 1
ISSN (Print): 2029-9990
Original language: English
Heat pump, Heat transfer, Magnetic refrigeration, Magnetocaloric effect, Test device modelling
Electronic versions:
15927_46878_1_PB.pdf
DOIs:
10.5755/j01.sace.14.1.15927
Fuel Cells and Electrolyzers. Recent Progress at DTU Energy and the Role in a Sustainable Society

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Aili, D. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Bibliographical note
Invited oral presentation

Functional Independent Scaling Relation for ORR/OER Catalysts
A widely used adsorption energy scaling relation between OH* and OOH* intermediates in the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), has previously been determined using density functional theory and shown to dictate a minimum thermodynamic overpotential for both reactions. Here, we show that the oxygen-oxygen bond in the OOH* intermediate is, however, not well described with the previously used class of exchange-correlation functionals. By quantifying and correcting the systematic error, an improved description of gaseous peroxide species versus experimental data and a reduction in calculational uncertainty is obtained. For adsorbates, we find that the systematic error largely cancels the vdW interaction missing in the original determination of the scaling relation. An improved scaling relation, which is fully independent of the applied exchange-correlation functional, is obtained and found to differ by 0.1 eV from the original. This largely confirms that, although obtained with a method suffering from systematic errors, the previously obtained scaling relation is applicable for predictions of catalytic activity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, SLAC National Accelerator Laboratory
Authors: Christensen, R. (Intern), Hansen, H. A. (Intern), Dickens, C. F. (Ekstern), Nørskov, J. K. (Ekstern), Vegge, T. (Intern)
Number of pages: 7
Pages: 24910-24916
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 120
Issue number: 43
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
Generating the optimal magnetic field for magnetic refrigeration

In a magnetic refrigeration device the magnet is the single most expensive component, and therefore it is crucially important to ensure that an effective magnetic field as possible is generated using the least amount of permanent magnets. Here we present a method for calculating the optimal remanence distribution for any desired magnetic field. The method is based on the reciprocity theorem, which through the use of virtual magnets can be used to calculate the optimal remanence distribution. Furthermore, we present a method for segmenting a given magnet design that always results in the optimal segmentation, for any number of segments specified. These two methods are used to determine the optimal magnet design of a 12-piece, two-pole concentric cylindrical magnet for use in a continuously rotating magnetic refrigeration device.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Insinga, A. R. (Intern), Smith, A. (Intern), Bahl, C. (Intern)
Number of pages: 4
Publication date: 2016
Globally Optimal Segmentation of Permanent-Magnet Systems

Permanent-magnet systems are widely used for generation of magnetic fields with specific properties. The reciprocity theorem, an energy-equivalence principle in magnetostatics, can be employed to calculate the optimal remanent flux density of the permanent-magnet system, given any objective functional that is linear in the magnetic field. This approach, however, yields a continuously varying remanent flux density, while in practical applications, magnetic assemblies are realized by combining uniformly magnetized segments. The problem of determining the optimal shape of each of these segments remains unsolved. We show that the problem of optimal segmentation of a two-dimensional permanent-magnet assembly with respect to a linear objective functional can be reduced to the problem of piecewise linear approximation of a plane curve by perimeter maximization. Once the problem has been cast into this form, the globally optimal solution can be easily computed employing dynamic programming.

Graphene layer encapsulated metal nanoparticles as a new type of non-precious metal catalysts for oxygen reduction

Cheap and efficient non-precious metal catalysts for oxygen reduction have been a focus of research in the field of low-temperature fuel cells. This review is devoted to a brief summary of the recent work on a new type of catalysts, i.e., the graphene layer encapsulated metal nanoparticles. The discussion is focused on the synthesis, structure, mechanism, performance, and further research.
A gas permeable porous support is a crucial part of an asymmetric oxygen transport membrane (OTM). Here, we develop feedstocks for thermoplastic extrusion of tubular, porous 3Y-TZP (partially stabilized zirconia polycrystals, (Y$_2$O$_3$)$_{0.03}$(ZrO$_2$)$_{0.97}$) ceramics, using graphite and/or polymethyl methacrylate (PMMA) as pore formers. The influence of pore former content and type, 3Y-TZP particle size and support sintering temperature on the microstructure, porosity and gas permeability were studied. Using at least 40 vol% pore former, consisting of graphite and PMMA in the volume ratio 2:1,
tubes with gas permeability exceeding the target of $10^{-14}$ m$^2$ are obtained. In the temperature range 1250–1400°C the support gas permeability is insensitive to the sintering temperature, and the feedstocks shrink more than 15% during sintering, making them ideal for co-sintering with functional OTM layers. This demonstrates the suitability of thermoplastic extrusion for fabrication of porous 3Y-TZP OTM supports, or for other technologies requiring porous ceramics.

**General information**

**State:** Published
**Organisations:** Department of Energy Conversion and Storage, Ceramic Engineering & Science
**Authors:** Bjørnetun Haugen, A. (Intern), Gurauskis, J. (Intern), Kaiser, A. (Intern), Søgaard, M. (Intern)
**Number of pages:** 9
**Pages:** 1039-1047
**Publication date:** 2016
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** European Ceramic Society. Journal
**Volume:** 37
**Issue number:** 3
**ISSN (Print):** 0955-2219
**Ratings:**
  - BFI (2018): BFI-level 1
  - BFI (2017): BFI-level 1
  - Web of Science (2017): Indexed Yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 1.392 SNIP 1.945
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 1
  - Scopus rating (2009): SJR 1.381 SNIP 1.724
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 1.146 SNIP 1.645
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 1.22 SNIP 1.76
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.191 SNIP 1.67
  - Web of Science (2006): Indexed yes
Graphitic Layer Encapsulated Iron Based Non-precious Catalysts for the Oxygen Reduction Reaction

Proton exchange membrane fuel cells (PEMFCs) are highly efficient energy conversion devices, which can be in combination with hydrogen fuel providing a clean energy technology to produce electricity. One crucial challenge for this technology is the large cathodic overpotential due to the sluggish oxygen reduction reaction (ORR) kinetics. Carbon supported platinum (Pt/C) is the state-of-the-art benchmarking catalyst for PEMFCs since it exhibits the highest activity. However, the high cost and low abundance of noble metals have limited large-scale commercialization of the technology. Current efforts are made to develop non-precious metal catalysts (NPMCs) as a replacement to the Pt/C electrocatalysts. In this thesis, a new type of NPMCs is synthesized by means of a dry autoclave with volatile ferrocene and cyanamide as precursors. The catalysts are morphologically featured by porous microspheres consisting of uniform metallic nanoparticles encapsulated in graphitic layers. The thesis work is conducted aiming at three major objectives: further optimization of the pyrolysis to achieve improved performance of catalysts, investigation of the complex Fe-containing components, and exploration of the possible active sites.

By systematic investigation of pyrolytic parameters i.e. temperature and duration, the best performance is achieved at 700°C and 75 minutes, exhibiting a high catalytic activity in acid media (0.1 M HClO₄) with an onset potential of 0.85 V at 0.1 mA cm⁻² and a mass specific kinetic current of 7.84 A g⁻¹ at 0.7 V vs. RHE. A good stability with 25 mV potential losses after 10,000 cycles of potential scan between 0.6 and 1.0 V has also been demonstrated.

The featuring morphology of the catalysts, i.e. the porous microspheres consisting of the graphitic layer encapsulated metal-containing nanoparticles, is essentially maintained during the pyrolysis of varied durations and temperatures. The metal-containing nanoparticles showed changes in the iron phases and their contents, as characterized by ⁵⁷Fe Mössbauer spectroscopy. The iron containing components include reduced metals (α-Fe and γ-Fe), oxide (γ-Fe₂O₃), carbide (Fe₃C) as well as a minor paramagnetic component due to Fe³⁺ (high spin) and/or possibly Fe²⁺ (low spin), likely coordinated with nitrogen (FeNx/C) as well identified for the Fe/N/C type catalysts in the literatures.

Quantitative determination of these metal containing components by low temperature ⁵⁷Mössbauer spectra shows that the content of the reduced metal component is steadily increasing with the pyrolytic time and temperature while the content of iron oxide is nearly constant. The most interesting finding is that the Fe³C content shows a peak in both the temperature-varying and the duration-varying series of samples. The possible FeNx/C coordination phase, however, varies to a very limited extent for the studied samples.

The catalytic activities and mechanisms for ORR are evaluated by rotating disk electrode (RDE) and rotating ring-disk electrode (RRDE) voltammetry. In terms of the mass specific kinetic current density and half-wave potential, a strong correlation of the catalytic activity is established with the Fe³C content within the entire composition range from 1.1 wt% to 4.5 wt% as well as with the FeNx/C content in a narrow range from 0.5 wt% to 0.85 wt%. Other iron containing components, i.e. α-Fe, γ-Fe and Fe₂O₃, showed no association with the ORR activity. It is concluded that, for the present catalysts, the recognized encapsulated iron carbide is most likely contributing to the ORR catalysis, in addition to the well identified N-coordinated Fe species.

More evidences are found from the catalyst synthesized from nitrogen free precursors. This catalyst, consisting of only carbon encapsulated iron-based nanoparticles, shows some, though low, ORR activity, which is enhanced by the post heat treatment in an ammonia atmosphere, indicating the contribution of the nitrogen functionalities.

Two anions in the electrolyte are used to probe the iron containing active sites towards the ORR, cyanide (CN⁻) in alkaline and thiocyanate (SCN⁻) in acidic medium, which seem supporting the above conclusions. These findings provide new insights to the encapsulation structure of Fe based nanocatalysts and therefore options for further development of
Guanidinium nonaflate as a solid-state proton conductor

Protonic organic ionic plastic crystals (POIPCs) are a type of novel solid-state proton conductors. In this work, guanidinium nonaflate ([Gdm-H][NfO]) is reported to be a model POIPC. Its structure-property relationship has been investigated comprehensively. Infrared analysis of [Gdm-H][NfO] and its deuterated analogue [Gdm-D][NfO] confirms the complete formation of the proton salts. The cations in as-prepared [Gdm-D][NfO] are estimated to consist of $[\text{C}((\text{ND}_2)_2(\text{NH}_2))^{+}$ and $[\text{C}((\text{ND}_2)_3]^{+}$ with a molar ratio of around 1:1. The deuteration also proves that each guanidinium cation has six displaceable protons. Thermogravimetric analysis demonstrates that [Gdm-H][NfO] exhibits superior thermal stability in both nitrogen and air atmospheres. Isothermogravimetric analysis reveals its negligible vapor pressure with an estimated high enthalpy of vaporization (120.9 kJ mol$^{-1}$). Differential scanning calorimetry measurements of [Gdm-H][NfO] show four evident endothermic peaks prior to its melting transition at 186.2 °C with a low entropy of melting (17.70 J K$^{-1}$ mol$^{-1}$).

Shortly before the onset temperature of melting transition (186.2 °C), partial melting (partial liquefaction) was observed via polarized optical microscopy in the temperature region of 176-186 °C while the reason for partial melting of ionic plastic crystals is not clear yet. Variable-temperature powder X-ray diffraction tests confirm the related solid-solid phase transitions and demonstrate that [Gdm-H][NfO] exhibits short-range disorder and long-range positional order in the plastic crystalline phases. Dielectric spectroscopy measurements show that its ionic conductivity reaches $2.1 \times 10^{-3}$ S cm$^{-1}$ at 185 °C. The proton conduction in the plastic crystalline phases of [Gdm-H][NfO] is assumed to happen via the vehicle mechanism. In the molten state, the proton conduction follows a combination of the vehicle mechanism and the Grotthuss mechanism (structural diffusion). In summary, due to their exceptional physicochemical properties, POIPCs like [Gdm-H][NfO] are promising electrolyte materials for high temperature (100-200 °C) proton exchange membrane fuel cells. In addition, POIPC-based solid-state proton conductors are also expected to find applications in sensors and other electrochemical devices.
High Current Printed Transistor

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern), Schmidt, T. M. (Intern), Hösel, M. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 1
Pages: 28
Publication date: 2016

Host publication information
Title of host publication: Book of Abstracts. General Assembly of the Marie Curie Alumni Association 2016
Publisher: Marie Curie Alumni Association
Main Research Area: Technical/natural sciences
Conference: General Assembly of the Marie Curie Alumni Association, Venice, Italy, 04/03/2016 - 04/03/2016
Electronic versions:
High_Current_Printed_Transistor.pdf
Source: PublicationPreSubmission
Source-ID: 127807214
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

High Current Printed Transistor: Roll-to-Roll Manufacture and Thermal Behavior

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern), Schmidt, T. M. (Intern), Hösel, M. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from EMRS Spring Meeting 2016, Lille, France.
Main Research Area: Technical/natural sciences
Electronic versions:
High_Current_Printed_Transistor_emrs.pdf
Source: PublicationPreSubmission
Source-ID: 127807028
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
High Current Temperature Sensitive RolltoRoll Printed Transistor

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
High_Current_Temperature.pdf

Bibliographical note
Symposium PM4 : Novel Materials, Fabrication Routes and Devices for Environmental Monitoring
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

High ionic conductivity in confined bismuth oxide-based heterostructures
Bismuth trioxide in the cubic fluorite phase (δ-Bi₂O₃) exhibits the highest oxygen ionic conductivity. In this study, we were able to stabilize the pure δ-Bi₂O₃ at low temperature with no addition of stabilizer but only by engineering the interface, using highly coherent heterostructures made of alternative layers of δ-Bi₂O₃ and Yttria Stabilized Zirconia (YSZ), deposited by pulsed laser deposition. The resulting [δ-Bi₂O₃=YSZ] heterostructures are found to be stable over a wide temperature range (500-750 °C) and exhibits stable high ionic conductivity over a long time comparable to the value of the pure δ-Bi₂O₃, which is approximately two orders of magnitude higher than the conductivity of YSZ bulk.

Highly Interactive Surfaces on Impregnated electrodes - an in operando Raman Spectroscopy Study

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science, Aarhus University
Authors: Sanna, S. (Intern), Esposito, V. (Intern), Christensen, M. (Ekstern), Pryds, N. (Intern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A P L Materials
Volume: 4
Article number: 121101
ISSN (Print): 2166-532X
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 1.889 SNIP 0.898 CiteScore 3.67
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.802 SNIP 1.055 CiteScore 3.76
Scopus rating (2014): SJR 1.525 SNIP 1.25 CiteScore 2.9
Original language: English
Electronic versions:
High_ionic_conductivity.pdf
DOIs:
10.1063/1.4971801

Bibliographical note
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Source: PublicationPreSubmission
Source-ID: 127758590
Publication: Research - peer-review › Journal article – Annual report year: 2016

Highly Interactive Surfaces on Impregnated electrodes - an in operando Raman Spectroscopy Study

General information
State: Published
Highly selective NOx reduction for diesel engine exhaust via an electrochemical system

It is challenging to reduce the nitrogen oxides (NOx) in diesel engine exhaust due to the inhibiting effect of excess oxygen. In this study, a novel electrochemical deNOx system was developed, which eliminated the need for additional reducing materials or a sophisticated controlling system as used in current diesel after-treatment techniques. The electrochemical system consisted of an electrochemical cell modified with NOx adsorbents and a diesel oxidation catalyst placed upstream of the cell. The system offers highly selective NOx reduction and a strong resistance to oxygen interference with almost zero emission of secondary pollutants.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, West Virginia University
Authors: Shao, J. (Intern), Tao, Y. (Ekstern), Kammer Hansen, K. (Intern)
Number of pages: 5
Pages: 36-40
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemistry Communications
Volume: 72
ISSN (Print): 1388-2481
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.53 SJR 1.618 SNIP 1.076
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.663 SNIP 1.2 CiteScore 4.77
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.848 SNIP 1.362 CiteScore 5.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.811 SNIP 1.435 CiteScore 4.97
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.315 SNIP 1.575 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.14 SNIP 1.615 CiteScore 5.14
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.181 SNIP 1.554
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.071 SNIP 1.552
High-performance membrane-electrode assembly with an optimal polytetrafluoroethylene content for high-temperature polymer electrolyte membrane fuel cells

Although high-temperature polymer electrolyte membrane fuel cells (HT-PEMFCs) have a high carbon monoxide tolerance and allow for efficient water management, their practical applications are limited due to their lower performance than conventional low-temperature PEMFCs. Herein, we present a high-performance membrane-electrode assembly (MEA) with an optimal polytetrafluoroethylene (PTFE) content for HT-PEMFCs. Low or excess PTFE content in the electrode leads to an inefficient electrolyte distribution or severe catalyst agglomeration, respectively, which hinder the formation of triple phase boundaries in the electrodes and result in low performance. MEAs with PTFE content of 20 wt% have an optimal pore structure for the efficient formation of electrolyte/catalyst interfaces and gas channels, which leads to high cell performance of approximately 0.5 A cm⁻² at 0.6 V.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Yonsei University, Korea Advanced Institute of Science & Technology, Korea Institute of Science and Technology
Authors: Jeong, G. (Ekstern), Kim, M. (Ekstern), Han, J. (Intern), Kim, H. (Ekstern), Shul, Y. (Ekstern), Cho, E. (Ekstern)
Number of pages: 5
Pages: 142-146
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 323
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
High-performance microchanneled asymmetric Gd$_{0.1}$Ce$_{0.9}$O$_{1.95-\delta}$-La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$-based membranes for oxygen separation

A microchanneled asymmetric dual phase composite membrane of 70 vol % Gd$_{0.1}$Ce$_{0.9}$O$_{1.95-\delta}$-30 vol % La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$ (CGO-LSF) was fabricated by a "one step" phase-inversion tape casting. The sample consists of a thin dense membrane (100 μm) and a porous substrate including "finger-like" microchannels. The oxygen permeation flux through the membrane with and without catalytic surface layers was investigated under a variety of oxygen partial pressure gradients. At 900 degrees C, the oxygen permeation flux of the bare membrane was 1.6 (STP) ml cm$^{-2}$ min$^{-1}$ for the air/He-case and 10.10 (STP) ml cm$^{-2}$ min$^{-1}$ for the air/CO-case. Oxygen flux measurements as well as electrical conductivity relaxation show that the oxygen flux through the bare membrane without catalyst is limited by the oxygen surface exchange. The surface exchange can be enhanced by introduction of catalyst on the membrane surface. An increase of the oxygen flux of 4.49 (STP) ml cm$^{-2}$ min$^{-1}$ at 900 degrees C was observed when catalyst is added for the air/He-case. Mass transfer polarization through the finger-like support was confirmed to be negligible, which
benefits the overall performance. A stable flux of 7.00 (STP) ml cm\(^{-2}\) min\(^{-1}\) was observed between air/CO/CO\(_2\) over 200 h at 850 degrees C. Partial surface decomposition was observed on the permeate side exposed to CO, in line with predictions from thermodynamic calculations. In a mixture of CO, CO\(_2\), H\(_2\), and H\(_2\)O at similar oxygen activity the material will according to the calculation not decompose. The microchanneled asymmetric CGO-LSF membranes show high oxygen permeability and chemical stability under a range of technologically relevant oxygen potential gradients.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Ceramic Engineering & Science, University of Science and Technology of China, Jilin University
Number of pages: 13
Pages: 4548-4560
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: A C S Applied Materials and Interfaces
Volume: 8
Issue number: 7
ISSN (Print): 1944-8244
Ratings:
  - BFI (2018): BFI-level 2
  - BFI (2017): BFI-level 1
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
  - ISI indexed (2011): ISI indexed no
  - Web of Science (2011): Indexed yes
  - Scopus rating (2010): SJR 1.571 SNIP 0.931
  - Web of Science (2010): Indexed yes
  - Web of Science (2009): Indexed yes
  - Original language: Undefined/Unknown
  - Phase inversion, Dual-phase composite membranes, Electrical conductivity relaxation, Surface exchange, Mass transfer polarization, Thermodynamic calculation

**DOIs:**

10.1021/acsami.5b10714

**Relations**

Projects:
- High-Performance Microchanneled Asymmetric Gd\(_{0.1}\)Ce\(_{0.9}\)O\(_{1.95-δ}\)-La\(_{0.6}\)Sr\(_{0.4}\)FeO\(_{3-δ}\)-Based Membranes for Oxygen Separation
High Performance Nano-Ceria Electrodes for Solid Oxide Cells

In solid oxide electrochemical cells, the conventional Ni-based fuel-electrodes provide high electrocatalytic activity but they are often a major source of long-term performance degradation due to carbon deposition, poisoning of reaction sites, Ni mobility, etc. Doped-ceria is a promising mixed ionic-electronic conducting oxide that could solve these issues if it can be integrated into an appropriate electrode structure. Two new approaches to obtain high-performance nanostructured doped-ceria electrodes are highlighted. The first is an infiltration-based architecture with Ce$_{0.8}$Pr$_{0.2}$O$_{2-\delta}$ forming the active surfaces on a porous backbone with embedded electronic current collector material, yielding one of the highest performances reported for an electrode that operates either on fuel or oxidant. The second is a nano-Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ thin film prepared by spin-coating, which provides an unprecedented electrode polarization resistance of ~0.01 Ω·cm$^2$ at 650 °C in H$_2$/H$_2$O. These results demonstrate that nano-ceria has the ability to achieve higher performance than Ni-based electrodes and show that the main challenge is obtaining sufficient electronic current collection without adding too much inactive material.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science
Authors: Graves, C. R. (Intern), Martinez Aguilera, L. (Intern), Sudireddy, B. R. (Intern)
Number of pages: 10
Pages: 183-192
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

Publication information

Journal: E C S Transactions
Volume: 72
Issue number: 7
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
High Temperature Alkaline Electrolysis Cells with Metal Foam Based Gas Diffusion Electrodes

Alkaline electrolysis cells operating at 250°C and 40 bar are able to convert electrical energy into hydrogen at very high efficiencies and power densities. In the present work we demonstrate the application of a PTFE hydrophobic network and Ag nanowires as oxygen evolution electrocatalyst in the metal foam based gas diffusion electrodes. A novel cell production method, based on tape casting and hot pressing, was developed which allows to increase the cell size from lab scale (1 cm$^2$) to areas of 25 cm$^2$ or larger. The thickness of the electrolyte matrix could be adjusted to only 200 μm, achieving a serial resistance and total area specific resistance of only 60 mΩ cm$^2$ and 150 mΩ cm$^2$, respectively, at 200°C and 20 bar, yielding a record high current density of 3.75 A cm$^{-2}$ at a cell voltage of 1.75 V. Encouraging long-term stability was obtained over 400 h of continuous electrolysis. This novel cell concept promises more than a 10-fold improvement in power density, compared to conventional alkaline electrolysis cells, and thereby equivalent reduction in stack size and cost.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Chatzichristodoulou, C. (Intern), Allebrod, F. (Intern), Mogensen, M. B. (Intern)
Number of pages: 5
Pages: F3036-F3040
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Journal
Volume: 163
Issue number: 11
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Moving away from fossil fuels requires harvesting more and more intermittent renewable energy resources and establishing a sustainable system for the production of chemicals. This brings forward the need for efficient large scale energy storage technologies and technologies for the conversion of renewable electricity to chemicals. Electrochemical reactors can play a crucial role in this endeavor, since they can efficiently and reversibly transform electricity to high-value chemicals, and thus serve as energy storage and recovery devices for balancing the grid, while offering a means for the sustainable production of chemicals.

A novel type of alkaline electrochemical cell that can operate at elevated temperature and pressure has been developed that relies on corrosion resistant high temperature diaphragms, based on mesoporous ceramic membranes where aqueous KOH is immobilized by capillary forces. Raising the operating temperature offers a means to boost performance, as both ionic transport and reaction kinetics are exponentially activated with temperature. Indeed, we have demonstrated alkaline electrolysis cells operating at 200-250 °C and 20-50 bar at very high efficiencies and power densities.

This work will provide an overview of our efforts to develop components of such high temperature alkaline electrochemical reactors for different applications. Low-cost large-scale production methods have been successfully employed for the production of ceramic diaphragms and full cells. The influence of composition and microstructure on the long-term chemical stability and mechanical durability of the mesoporous ceramic membranes has been explored. Instrumentation for electrochemical testing at elevated pressures (up to 99 bar) and temperatures (up to 300 °C) with in-line chemical analysis has been established enabling experiments with gaseous or liquids reactants/products at cell sizes of up to 25
cm2. Efforts are currently directed towards the investigation of the intrinsic activity of mixed oxides for the oxygen evolution reaction at elevated temperatures and pressures, and of the intrinsic activity, selectivity and stability of supported metal catalysts towards the electrocatalytic conversion of biomass derivatives to high-value chemicals. Finally, the use of selected electrocatalysts for the production of high performance electrodes will be reported.

**General information**
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Chatzichristodoulou, C. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3061
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/40/3061.abstract?sid=c6d3278d-159f-46a1-81f4-8f81c7ab155d
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

**High temperature conductance mapping for correlation of electrical properties with micron-sized chemical and microstructural features**
High temperature AC conductance mapping is a scanning probe technique for resolving local electrical properties in microscopic areas. It is especially suited for detecting poorly conducting phases and for ionically conducting materials such as those used in solid oxide electrochemical cells. Secondary silicate phases formed at the edge of lanthanum strontium manganese microelectrodes are used as an example for correlation of chemical, microstructural and electrical properties with a spatial resolution of 1–2 µm to demonstrate the technique. The measurements are performed in situ in a controlled atmosphere high temperature scanning probe microscope at 650°C in air.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry
Authors: Hansen, K. V. (Intern), Norrman, K. (Intern), Jacobsen, T. (Intern)
Number of pages: 8
Pages: 69-76
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Ultramicroscopy
Volume: 170
ISSN (Print): 0304-3991
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.82 SJR 1.915 SNIP 1.233
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.121 SNIP 1.428 CiteScore 2.78
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.638 SNIP 1.661 CiteScore 2.59
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.777 SNIP 1.337 CiteScore 2.66
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
High temperature in operando and in situ spectroscopy on electrified surfaces and interfaces

Electrochemical cells, such as fuel cells, electrolyzers and batteries are considered as important technologies for storing electricity from renewable sources and also provide an efficient way of converting chemical energy into electricity. The processes in the electrodes are strongly influenced by the surface electrocatalytic properties, especially if instead of (or in addition to) hydrogen more complex reactants such hydrocarbons in form of alcohols, methane or higher hydro carbons are used as reactants. High temperature, solid state electrochemical cells based on an oxide ion conducting electrolyte are particularly attractive since hydrocarbon fuels in principle can be directly converted into electricity and vice versa with high efficiency. However, several side effects such as coking and poisoning with impurities e.g. sulfur on the fuel electrode, but also indication of changes in surface chemistry of oxide electrodes without contaminants have demanded a better insight into the electrode surface reactions and chemistries. Spectroscopic techniques can be applied to these cells but are still experimentally challenging due to the high temperature operation conditions. DTU Energy has in the recent years invested in specific equipment that allows investigating the electronic, electrical and chemical structure of surfaces under polarization at high temperatures and controlled atmospheres, allowing investigation of electrochemical cells and interfaces under close to operation conditions. The contribution will present selected examples of Raman spectroscopy, Kelvin probe and scanning probe microscopy applied to solid oxide electrochemical cells.
High temperature polymer electrolyte membrane fuel cells: Approaches, status, and perspectives
This book is a comprehensive review of high-temperature polymer electrolyte membrane fuel cells (PEMFCs). PEMFCs are the preferred fuel cells for a variety of applications such as automobiles, cogeneration of heat and power units, emergency power and portable electronics. The first 5 chapters of the book describe rationalization and illustration of approaches to high temperature PEM systems. Chapters 6 - 13 are devoted to fabrication, optimization and characterization of phosphoric acid-doped polybenzimidazole membranes, the very first electrolyte system that has demonstrated the concept of and motivated extensive research activity in the field. The last 11 chapters summarize the state-of-the-art of technological development of high temperature-PEMFCs based on acid doped PBI membranes including catalysts, electrodes, MEAs, bipolar plates, modelling, stacking, diagnostics and applications.

Homogenization of steady-state creep of porous metals using three-dimensional microstructural reconstructions
The effective steady-state creep response of porous metals is studied by numerical homogenization and analytical modeling in this paper. The numerical homogenization is based on finite element models of three-dimensional microstructures directly reconstructed from tomographic images. The effects of model size, representativeness, and boundary conditions on the numerical results are investigated. Two analytical models for creep rate of porous bodies are derived by extending the Hashin-Shtrikman bound and the Ramakrishnan-Arunchalam model in linear elasticity to steady-state creep based on nonlinear homogenization. The numerical homogenization prediction and analytical models obtained in this work are compared against reported measurements and models. The relationship between creep rate and porosity computed by homogenization is found to be bounded by the Hodge-Dunand model and the Hashin-Shtrikman creep model, and closely matched by the Gibson-Ashby compression and the Ramakrishnan-Arunchalam creep models. [All rights reserved Elsevier].

Mixed Conductors
The effective steady-state creep response of porous metals is studied by numerical homogenization and analytical modeling in this paper. The numerical homogenization is based on finite element models of three-dimensional microstructures directly reconstructed from tomographic images. The effects of model size, representativeness, and boundary conditions on the numerical results are investigated. Two analytical models for creep rate of porous bodies are derived by extending the Hashin-Shtrikman bound and the Ramakrishnan-Arunchalam model in linear elasticity to steady-state creep based on nonlinear homogenization. The numerical homogenization prediction and analytical models obtained in this work are compared against reported measurements and models. The relationship between creep rate and porosity computed by homogenization is found to be bounded by the Hodge-Dunand model and the Hashin-Shtrikman creep model, and closely matched by the Gibson-Ashby compression and the Ramakrishnan-Arunchalam creep models. [All rights reserved Elsevier].
In situ diagnostics of the crystal-growth process through neutron imaging: application to scintillators

Neutrons are known to be unique probes in situations where other types of radiation fail to penetrate samples and their surrounding structures. In this paper it is demonstrated how thermal and cold neutron radiography can provide time-resolved imaging of materials while they are being processed (e.g. while growing single crystals). The processing equipment, in this case furnaces, and the scintillator materials are opaque to conventional X-ray interrogation techniques. The distribution of the europium activator within a BaBrCl:Eu scintillator (0.1 and 0.5% nominal doping concentrations per mole) is studied in situ during the melting and solidification processes with a temporal resolution of 5-7 s. The strong tendency of the Eu dopant to segregate during the solidification process is observed in repeated cycles, with Eu forming clusters on multiple length scales (only for clusters larger than ∼50 μm, as limited by the resolution of the present experiments). It is also demonstrated that the dopant concentration can be quantified even for very low concentration levels (∼ 0.1%) in 10 mm thick samples. The interface between the solid and liquid phases can also be imaged, provided there is a sufficient change in concentration of one of the elements with a sufficient neutron attenuation cross section. Tomographic imaging of the BaBrCl:0.1% Eu sample reveals a strong correlation between crystal fractures and Eu-deficient clusters. The results of these experiments demonstrate the unique capabilities of neutron imaging for in situ diagnostics and the optimization of crystal-growth procedures.
In situ time-of-flight neutron imaging of NiO-YSZ anode support reduction under influence of stress

This article reports on in situ macroscopic scale imaging of NiO-YSZ (YSZ is yttria-stabilized zirconia) reduction under applied stress - a phase transition taking place in solid oxide electrochemical cells in a reducing atmosphere of a hydrogen/nitrogen mixture and at operation temperatures of up to 1073 K. This process is critical for the performance and lifetime of the cells. Energy-resolved neutron imaging was applied to observe the phase transition directly with time and spatial resolution. Two different approaches are presented for using this imaging technique for the investigation of chemical and physical processes requiring controlled atmosphere and elevated temperature. The first type of measurement is based on alternating stages of short-term partial chemical reaction and longer neutron image acquisition, and the second type is a real in situ neutron imaging experiment. Results of applying energy-resolved neutron imaging with both approaches to the NiO-YSZ reduction investigation indicate enhancement of the reduction rate due to applied stress, which is consistent with the results of the authors’ previous research.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, European Spallation Source ESS AB, Xnovo Technology ApS, Rutherford Appleton Laboratory, University of California at Berkeley
Authors: Makowska, M. G. (Intern), Strobl, M. (Ekstern), Lauridsen, E. M. (Ekstern), Kabra, S. (Ekstern), Kockelmann, W. (Ekstern), Tremsin, A. (Ekstern), Frandsen, H. L. (Intern), Kuhn, L. T. (Intern)
Number of pages: 8
Pages: 1674-1681
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 49
Issue number: 5
ISSN (Print): 0021-8898
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
In situ transmission electron microscopy for magnetic nanostructures

Nanomagnetism is a subject of great interest because of both application and fundamental aspects in which understanding of the physical and electromagnetic structure of magnetic nanostructures is essential to explore the magnetic properties. Transmission electron microscopy (TEM) is a powerful tool that allows understanding of both physical structure and micromagnetic structure of the thin samples at nanoscale. Among TEM techniques, in situ TEM is the state-of-the-art approach for imaging such structures in dynamic experiments, reconstructing a real-time nanoscale picture of the properties-structure correlation. This paper aims at reviewing and discussing in situ TEM magnetic imaging studies, including Lorentz microscopy and electron holography in TEM, applied to the research of magnetic nanostructures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of Manchester
Authors: Ngo, D. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 16
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advances in Natural Sciences: Nanoscience and Nanotechnology
Volume: 7
Issue number: 4
Article number: 045001
ISSN (Print): 2043-6254
In situ X-ray powder diffraction studies of the synthesis of graphene oxide and formation of reduced graphene oxide

Graphene oxide (GO) and reduced graphene oxide (rGO) are important materials in a wide range of fields. The modified Hummers methods, for synthesizing GO, and subsequent thermal reduction to rGO, are often employed for production of rGO. However, the mechanism behinds these syntheses methods are still unclear. We present an in situ X-ray diffraction study of the synthesis of GO and thermal reduction of GO. The X-ray diffraction revealed that the Hummers method includes an intercalation state and finally formation of additional crystalline material. The formation of GO is observed during both the intercalation and the crystallization stage. During thermal reduction of GO three stages were observed: GO, a disordered stage, and the rGO stage. The appearance of these stages depends on the heating ramp. The aim of this study is to provide deeper insight into the chemical and physical processes during the syntheses.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Storm, M. M. (Intern), Johnsen, R. E. (Intern), Norby, P. (Intern)
Number of pages: 6
Pages: 49-54
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Solid State Chemistry
Volume: 240
ISSN (Print): 0022-4596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
In situ X-ray scattering of perovskite solar cell active layers roll-to-roll coated on flexible substrates

In an effort to understand recent results showing differences between the power conversion efficiencies of lead halide (CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$) solar cells on glass versus flexible substrates, this study investigates the influence that substrate and processing methods have on morphological and crystallographic development. Using our in situ slot-die micro roll-to-roll
coater setup, we measured small and wide angle X-ray scattering in grazing incidence while the material dried, enabling us to follow the crystallization from just after the deposition and up to 25 minutes later. The data showed differing crystallographic developments between the substrates, especially seen through the behaviour of a crystalline precursor which survived longer on the flexible substrates than on glass. Additionally, the common degradation product PbI₂ was absent on the thickest flexible substrate. This leads us to conjecture that the flexible substrates absorb part of the solvent, thereby delaying evaporation and changing the solvent environment around the perovskite. As a further test, we produced solar cells with the same substrates and confirmed that the ones made on flexible substrates performed worse than those made on glass, but that when including an ITO layer in the stack it seemed to act as a buffer, whereby the solar cell performance was improved.

General information
State: Published
Number of pages: 6
Pages: 5083-5088
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: CrystEngComm
Volume: 18
Issue number: 27
ISSN (Print): 1466-8033
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 1.043 SNIP 0.904
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.063 SNIP 0.999 CiteScore 3.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.131 SNIP 1.11 CiteScore 3.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.079 SNIP 1.11 CiteScore 3.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.253 SNIP 1.142 CiteScore 3.83
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.174 SNIP 1.191 CiteScore 3.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.233 SNIP 1.229
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.227 SNIP 1.257
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.297 SNIP 1.183
Scopus rating (2007): SJR 1.42 SNIP 1.704
Impact of Prosumer Buildings and their Clusters on the Energy System – project outline

General information
State: Published
Organisations: Department of Civil Engineering, Section for Building Energy, Department of Energy Conversion and Storage
Authors: Larma, M. (Intern), Heller, A. (Intern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Implementation of Constrained DFT for Computing Charge Transfer Rates within the Projector Augmented Wave Method
Combining constrained density function theory (cDFT) with Marcus theory is an efficient and promising way to address charge transfer reactions. Here, we present a general and robust implementation of cDFT within the projector augmented wave (PAW) framework. PAW pseudopotentials offer a reliable frozen-core electron description across the whole periodic table, with good transferability, as well as facilitate the extraction of all-electron quantities. The present implementation is applicable to two different wave function representations, atomic-centered basis sets (LCAO) and the finite-difference (FD) approximation utilizing real-space grids. LCAO can be used for large systems, molecular dynamics, or quick initialization, while more accurate calculations are achieved with the FD basis. Furthermore, the calculations can be performed with flexible boundary conditions, ranging from isolated molecules to periodic systems in one-, two-, or three-dimensions. As such, this implementation is relevant for a wide variety of applications. We also present how to extract the electronic coupling element and reorganization energy from the resulting diabatic cDFT-PAW wave functions for the parametrization of Marcus theory. Here, the combined method is applied to important test cases where practical implementations of DFT fail due to the self-interaction error, such as the dissociation of the helium dimer cation, and it is compared to other established cDFT codes. Moreover, for charge localization in a diamine cation, where it was recently shown that the commonly used generalized gradient and hybrid functionals of DFT failed to produce the localized state, cDFT produces qualitatively and quantitatively accurate results when benchmarked against self-interaction corrected DFT and high-level CCSD(T) calculations at a fraction of the computational cost.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Center for Atomic-scale Materials Design, Department of Physics, Aalto University
Authors: Melander, M. (Intern), Jönsson, E. Ö. (Ekstern), Mortensen, J. J. (Intern), Vegge, T. (Intern), García Lastra, J. M. (Intern)
Number of pages: 12
Pages: 5367-5378
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Theory and Computation
Improved electrodes and gas impurity investigations on alkaline electrolysers
Alkaline water electrolysis for hydrogen production is a well-established technique, but some technological issues regarding the coupling of alkaline water electrolysis and Renewable Energy Sources (RES) remain to be improved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, German Aerospace Center, Flemish Institute for Technological Research, Hydrogenics Europe NV
Number of pages: 1
Publication date: 2016
Event: Poster session presented at The 21st World Hydrogen Energy Conference (WHEC), Zaragoza, Spain.
Improving the Operational Stability of PBDTTTz-4 Polymer Solar Cells Modules by Electrode Modification

PBDTTTz-4 is employed in the ambient manufacturing of fully Roll-to-Roll organic solar cell modules. Modules are manufactured using a novel silver nanowire electrode or a previously reported carbon electrode. The average PCE of carbon modules (3.07%) and AgNW modules (1.46%) shows that PBDTTTz-4 is a good candidate for upscaling. Stability measurements following the ISOS standards are used to compare the lifetime of the different modules. In all tests but one, the carbon modules are less stable. The higher stability of AgNW is attributed to the removal of the PEDOT:PSS in the front electrode. Finally during indoor light tests, a new degradation phenomenon is observed where bubbles are formed inside the modules contrary to previous reports of bubble formation by thermal expansion of trapped gas inside the barrier.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 7
Pages: 511-517
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Advanced Engineering Materials
Volume: 18
Issue number: 4
ISSN (Print): 1438-1656
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.826 SNIP 1.083
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.807 SNIP 1.045 CiteScore 1.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.805 SNIP 1.089 CiteScore 1.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.733 SNIP 0.843 CiteScore 1.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.779 SNIP 0.959 CiteScore 1.46
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.828 SNIP 1.035 CiteScore 1.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.097 SNIP 1.14
BFI (2009): BFI-level 1
Improving the performance of district heating systems by utilization of local heat boosters

District Heating (DH) plays an important role into the Danish energy green transition towards the future sustainable energy systems. The new, 4th generation district heating network, the so called Low Temperature District Heating (LTDH), tends to lower the supply temperature of the heat down to 40-50°C with return temperatures of 20-30 °C. This kind of heating system has many advantages and among all of them, it allows utilization of the heat coming from low exergy heat sources, as well as to decrease the grid heat losses. Electrical energy driven heat sources are also integrated into the future LTDH grid as they will have the strategical role of connecting the heating system with the electrical energy coming from the intermittent and fluctuating renewable energy sources such as wind and solar power. In this paper a case study of district heating system is presented and analysed. The goal was to evaluate the possibilities to lower the forward temperature of the heat supply in order to reduce the heat losses of the system. Booster heat pumps are introduced to increase the water temperature close to the final users. A Matlab model was developed to simulate the state of the case study DH network in terms of mass flow rates, temperatures and heat losses. After the model simulation, a new configuration of district heating with the introduction of three booster heat pumps was proposed. The new system’s operation is determined based on a non-linear optimization problem in which the objective function was set to minimize the system heat losses.

Corresponding author 0303-1 1 This goal was achieved by lowering the forward temperature to 40°C and relying on the installed heat pumps to boost the water temperature to the admissible value needed for the domestic hot water preparation. Depending on the season, the optimized configuration allows decreasing the network heat losses in the range of 38-54%, higher reductions being achieved during colder seasons.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Sapienza University of Rome
Authors: Falcone, A. (Ekstern), Dominkovic, D. F. (Intern), Pedersen, A. S. (Intern)
Number of pages: 21
Publication date: 2016
Main Research Area: Technical/natural sciences
DOIs:
10.6084/m9.figshare.4595515.v1
Source: PublicationPreSubmission
Source-ID: 131716569
Publication: Research - peer-review › Paper – Annual report year: 2017
Incineration of organic solar cells: Efficient end of life management by quantitative silver recovery

Recovery of silver from the electrodes of roll-to-roll processed organic solar cells after incineration has been performed quantitatively by extraction with nitric acid. This procedure is more than 10 times faster than previous reports and the amount of acid needed for the extraction is reduced by a factor of 100-150. LCA studies show that the resulting environmental impacts from silver extraction of incinerated ashes are more favourable on almost all standard factors compared to extraction from shredded organic solar cells. The so lessened environmental impacts by efficient recovery fully justify the use of Ag as an electrode in scaled production of organic solar cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Applied Sciences and Arts Northwestern Switzerland
Authors: Søndergaard, R. R. (Intern), Zimmermann, Y. S. (Ekstern), Espinosa Martinez, N. (Intern), Lenz, M. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 5
Pages: 857-861
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 9
Issue number: 3
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 10.027 SNIP 4.275 CiteScore 23.85
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.792 SNIP 4.034 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.02 SNIP 3.011 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.86 SNIP 2.594 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.743 SNIP 2.513 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.861 SNIP 2.41
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.045 SNIP 1.139
Original language: English
Electronic versions:
c6ee00021e.pdf
DOIs:
10.1039/c6ee00021e

Bibliographical note
Infiltration of SOFC Stacks: Evaluation of the Electrochemical Performance Enhancement and the Underlying Changes in the Microstructure

Experimental SOFC stacks with 10 SOFCs (LSM-YSZ/YSZ/Ni-YSZ) were infiltrated with CGO and Ni-CGO on the air and fuel side, respectively in an attempt to counter degradation and improve the output. The electrochemical performance of each cell was characterized (i) before infiltration, (ii) after infiltration on the cathode side, and (iii) after the infiltration of the anode side. A significant performance enhancement was observed after the infiltration with CGO on the cathode, while the infiltration of the anode side with Ni-CGO had no significant effect on the electrochemical performance. After testing the cells were characterized by SEM and TEM/EELS. A thin layer of CGO nanoparticles around the LSM-YSZ backbone structure was found after infiltration. On the anode side nano sized Ni particles were found embedded in a CGO layer formed around the Ni-YSZ structure. EELS analysis showed that the oxidation state of the Ce ions is identical on the air and the fuel side.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry, Imaging and Structural Analysis, Case Western Reserve University, Topsoe Fuel Cell
Number of pages: 9
Pages: 80-88
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 16
Issue number: 1
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.699 SNIP 0.787 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.629 SNIP 0.816 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.841 SNIP 0.848 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.25 SNIP 1.008 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.656 SNIP 1.238 CiteScore 3.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Influence of pore former on porosity and mechanical properties of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ electrolytes for flue gas purification

Single layered porous Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ electrolytes were fabricated by tape casting using different types, shapes and sizes of pore formers and their respective strength and stiffness were compared. The sintered bodies were characterized by scanning electron microscopy, mercury porosimetry, impulse excitation technique (Young modulus) and flexural strength measurements, to investigate the role of the different pore formers on the properties of the compounds. The compared techniques used to evaluate porosity give consistent results. The ratio between open and total porosities, evaluated from mercury porosimetry, varies depending on the used pore formers. The stiffness and strength of the compounds show an exponential dependency to the total porosity. By considering the open porosity instead (functional porosity), we observe that samples with platelets shaped pore formers have higher in-plane strength than spherical pore formers. An optimum can be found in term of Weibull strength and strain of samples obtained with the various pore formers by considering the dependency on the functional open porosity instead of the total porosity.

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Influence of temperature and atmosphere on the strength and elastic modulus of solid oxide fuel cell anode supports

Solid Oxide Fuel Cells are subjected to significant stresses during production and operation. The various stress-generating conditions impose strength requirements on the cell components, and thus the mechanical properties of the critical load bearing materials at relevant operational conditions need to be characterized to ensure reliable operation. In this study, the effect of reduction temperature on microstructural stability, high temperature strength and elastic modulus of Ni-YSZ anode supports were investigated. The statistical distribution of strength was determined from a large number of samples (≈30) at each condition to ensure high statistical validity. It is revealed that the microstructure and mechanical properties of the Ni-YSZ strongly depend on the reduction temperature. Further studies were conducted to investigate the temperature dependence of the strength and elastic modulus for both the unreduced and reduced Ni(O)-YSZ anode supports. With increasing temperature, the strength and elastic modulus of the reduced Ni-YSZ specimens drop almost linearly. In contrast, the strength and elastic modulus of the unreduced NiO-YSZ remain almost constant over the investigated temperature range. Compared to the NiO-YSZ, a significantly lower strength and elastic modulus of the reduced Ni-YSZ is observed; while reduction leads to a remarkable increase in failure strain of the anode support.
Infrared ellipsometry study of the confined electrons in a high-mobility γ-Al2O3/SrTiO3 heterostructure

With infrared ellipsometry we studied the response of the confined electrons in γ-Al2O3/SrTiO3 (GAO/STO) heterostructures in which they originate predominantly from oxygen vacancies. From the analysis of a so-called Berreman mode, that develops near the highest longitudinal optical phonon mode of SrTiO3, we derive the sheet carrier density, Ns, the mobility, μ, and the depth profile of the carrier concentration. Notably, we find that Ns and the shape of the depth profile are similar as in LaAlO3/SrTiO3 (LAO/STO) heterostructures for which the itinerant carriers are believed to arise from a polar discontinuity. Despite an order of magnitude higher mobility in GAO/STO, as obtained from transport measurements, the derived mobility in the infrared range exhibits only a twofold increase. We interpret this finding in terms of the polaronic nature of the confined charge carriers in GAO/STO and LAO/STO which leads to a strong, frequency-dependent interaction with the STO phonons.
In Situ Analysis of the Li-O₂ Battery with Thermally Reduced Graphene Oxide Cathode: Influence of Water Addition

The Li-O₂ battery technology holds the promise to deliver a battery with significantly increased specific energy compared to today's Li-ion batteries. As a cathode support material, reduced graphene oxide has received increasing attention in the Li-O₂ battery community due to the possibility of increased discharge capacity, increased battery cyclability, and decreased charging overpotential. In this article we investigate the effect of water on a thermally reduced graphene oxide cathode in a Li-O₂ battery. Differential electrochemical mass spectrometry reveals a decreased electron count for batteries with 1000 ppm water added to the electrolyte in comparison to dry batteries, indicating additional parasitic electrochemical or chemical processes. A comparable capacity of the wet and dry batteries indicates that the reaction mechanism in the Li-O₂ battery also depends on the surface of the cathode and not only on addition of water to the electrolyte as demonstrated by the solution-based mechanism In situ synchrotron X-ray diffraction experiment using a new design of a capillary-based Li-O₂ cell with a thermally reduced graphene oxide cathode shows formation of LiOH along with Li₂O₂.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Uppsala University
In-situ, long-term operational stability of organic photovoltaics for off-grid applications in Africa

This paper presents a field-trial of organic photovoltaic (OPV) technology used within a practical application for rural electrification in Rwanda. Fourteen, large area, flexible, ITO-free, roll-to-roll processed OPV modules, encapsulated with low-cost materials, were installed on corrugated steel roofs at two sites in a rural village in Southern Rwanda and subject to continuous monitoring. This field-trial exposed modules to very high levels of insolation, in particular in the UV, high temperatures and heavy rainfall. Results show that the modules exhibit practical lifetimes (to degrade by 20% of their initial capacity) of between 2 and 5 months, a value 5-6 times lower than control modules kept both in the dark and outdoors in Roskilde, Denmark. Degradation was primarily the result of extensive delamination caused by failure of the non-UV stable encapsulation, which led to decay in the FF, Voc and Isc of the module.
In-situ SEM electrochemistry and radiolysis

Electron microscopy is a ubiquitous technique to see effects which are too small to see with traditional optical microscopes. Recently it has become possible to also image liquid samples by encapsulating them from the vacuum of the microscope and a natural evolution from that has been to include microelectrodes on the windows to enable studies of electrochemical processes. In this way it is possible to perform in-situ electrochemical experiments such as electroplating and charge and discharge analysis of battery electrodes.
In a typical liquid cell, electrons are accelerated to sufficiently high energies to traverse a thin window made by a silicon nitride membrane, and interact with the sample immersed in liquid. In transmission electron microscopy (TEM) the majority of the electrons continue through the sample to form an image. In scanning electron microscopy (SEM) a fraction of the electrons are backscattered and an image is reconstructed by the microscope. But the high energy electrons are a form of ionising radiation which can significantly affect the chemistry in liquid experiments. Ionising radiation can split water, produce radicals, reduce dissolved metal ions to metal particles, and more. It is therefore essential to understand and control the radiolytic processes that results from in-situ electron microscopy experiments.

Although radiolysis has been studied extensively in connection with the advent of e.g. nuclear reactors the information obtained for that purpose often has to be extrapolated many orders of magnitude to reach the radiation conditions of the extremely focused beam of typical electron microscopes. To date there is a distinct lack of direct measurements and quantification of the radiolytic conditions for in in-situ liquid cells.

In this thesis an electrochemical in-situ SEM cell is used to study the radiolytic effects of the electron beam. Potentiometric measurements in-situ demonstrate that the electrolyte contains hydrogen upon irradiation, and that the ratio of H₂O₂ to H₂ is only 1:2.5, much less than the predicted ratio of 1:1.1. Electrochemical impedance spectroscopy (EIS) measurements between two electrodes when irradiating at an average intensity of 6 MGy/s indicate that the conductivity may be at least 200 μS/cm, two orders of magnitude higher than what would be expected from H⁺ alone. Finally, the radiolytic yield of copper is measured by gradually increasing the radiation intensity until copper precipitated. Based on the amount of backscattered electrons it has been possible to quantify the amount of reduced copper, resulting in an average radiolytic yield per 100 eV of deposited energy (g-value) of 0.05, lower than the value of 4.4 seen in pulse radiolysis experiments. During the course of these studies it has also been possible to improve on the EC-SEM system. This has resulted in pyrolysed carbon electrodes, which offer the benefit of stability at 0.75 V higher potentials than traditional gold thin-film electrodes.

With the quantitative insight into the radiolytic conditions in liquid electron microscopy cells that this thesis provides it may be possible to design and analyse experiments where such effects are correctly accounted for. The results are therefore of high value for the in-situ community who until now have had to rely on only limited experimental data in combination with theoretical predictions that have been extrapolated several orders of magnitude.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Molecular Windows, Department of Energy Conversion and Storage, Center for Electron Nanoscopy
Authors: Møller-Nilsen, R. E. R. (Intern), Mølhave, K. (Intern), Norby, P. (Intern), Wagner, J. B. (Intern)
Number of pages: 112
Publication date: 2016

Publication information
Publisher: DTU Nanotech
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
ROLF_MOLLERNILSEN_Phd_Thesis_1.pdf

Relations
Projects:
In SITU Transmission Electron Microscopy on Operating Electrochemical CELLS
Source: PublicationPreSubmission
Source-ID: 127629530
Publication: Research › Ph.D. thesis – Annual report year: 2016

In SITU Transmission Electron Microscopy on Operating Electrochemical CELLS
Solid oxide cells (SOC) have the potential of playing a significant role in the future efficient energy system scenario. In order to become widely commercially available, an improved performance and durability of the cells has to be achieved [1]. Conventional scanning and transmission SEM and TEM have been often used for ex-situ post mortem characterization of SOFCs and SOECs [2,3]. However, in order to get fundamental insight of the microstructural development of SOFC/SOEC during operation conditions in situ studies are necessary [4].

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Fundamental Electrochemistry, Department of Micro- and Nanotechnology, Molecular Windows, Electrofunctional materials, Center for Electron Nanoscopy, Nagoya University
Authors: Gualandris, F. (Intern), Simonsen, S. B. (Intern), Mogensen, M. B. (Intern), Mølhave, K. (Intern), Sanna, S. (Intern), Wagner, J. B. (Intern), Muto, S. (Ekstern), Higuchi, K. (Ekstern), Kuhn, L. T. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Interface-Induced Renormalization of Electrolyte Energy Levels in Magnesium Batteries

A promising strategy for increasing the energy density of Li-ion batteries is to substitute a multivalent (MV) metal for the commonly used lithiated carbon anode. Magnesium is a prime candidate for such a MV battery due to its high volumetric capacity, abundance, and limited tendency to form dendrites. One challenge that is slowing the implementation of Mg-based batteries, however, is the development of efficient and stable electrolytes. Computational screening for molecular species having sufficiently wide electrochemical windows is a starting point for the identification of optimal electrolytes. Nevertheless, this window can be altered via interfacial interactions with electrodes. These interactions are typically omitted in screening studies, yet they have the potential to generate large shifts to the HOMO and LUMO of the electrolyte components. The present study quantifies the stability of several common electrolyte solvents on model electrodes of relevance for Mg batteries. Many-body perturbation theory calculations based on the G0W0 method were used to predict shifts in a solvent's electronic levels arising from interfacial interactions. In molecules exhibiting large dipole moments, our calculations indicate that these interactions reduce the HOMO-LUMO gap by ∼25% (compared to isolated molecules). We conclude that electrode interactions can narrow an electrolyte's electrochemical window significantly, thereby accelerating redox decomposition reactions. Accounting for these interactions in screening studies presents an opportunity to refine predictions of electrolyte stability.
In the chemical solution deposition process of YBCO superconducting films, fluorine is widely regarded to be of significant importance in avoiding the formation of BaCO3, which hinders the growth of high-quality YBCO films. On the other hand, great efforts have been made to decrease the fluorine content in the precursor solution due to the environmental contaminations of the fluorinated gaseous by-products. In this study, we demonstrate that an F/Ba atomic ratio of 2 in the precursor solution is sufficient according to the results of energy dispersive spectrometry and attenuated Fourier transform infrared studies. The intermediate phase evolution prior to the end of the sintering stage is also investigated by X-ray diffractometry and scanning electron microscopy. Liquid-like structures are observed, which are proposed to be responsible for the film densification in the early stage of YBCO formation. The formation of YBCO is accompanied by the consumption of oxygen-doped BaF2 (BOF), which is found to be highly textured. Moreover, in the early stage of YBCO formation, the crystallinity and texture of BOF enhance despite its consumption. After a full heat treatment, YBCO films with Jc of 5 MA/cm² (77 K, 0 T) could be routinely obtained on lanthanum aluminate single-crystal substrates.
Introduction

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hjuler, H. A. (Intern), Aili, D. (Intern), Li, Q. (Intern)

Chemical solution deposition, Fluorine, Intermediate phases, Thin films, YBCO

DOI: 10.1109/TASC.2016.2542273
Source: FindIt
Source-ID: 277452705
Publication: Research - peer-review › Journal article – Annual report year: 2016
Introduction to the Issue on Organic Nanophotonics

The papers in this special issue focus on the topic of organic nanophotonics. Since early works in the 1980s, significant advances have been made in organic materials with semiconducting and photonic properties due to the development of materials/device technologies on the nanoscale. The most impressive outcomes include organic light-emitting devices (OLEDs) that are now competing with the well-established liquid crystal display technology in the mobile and television markets. In addition, organic solar cells (OSCs) offer the potential to create new paradigms for ultrathin and lightweight plastic solar modules in the coming flexible electronics era. Further developments are ongoing across a broad range of organic nanophotonics topics including organic laser devices, organic phototransistors, organic plasmonic devices, etc.

This issue introduces recent cutting-edge research from the fast-breaking area of organic nanophotonics. The subject in this special issue includes organic lasers, OLEDs, organic photovoltaics, organic phototransistors, microcavities, and related materials. In particular, most papers included in this special issue offer insights into technology innovations including flexible optoelectronics. We trust that readers will benefit from the timely and in-depth research presented in this special issue and get an insight into future nanophotonics directions with organic and related materials.

General Information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Kyungpook National University, University of Oxford, Beijing Jiaotong University, Monash University
Number of pages: 3
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: IEEE Journal on Selected Topics in Quantum Electronics
Volume: 22
Issue number: 1
Article number: 0200103
ISSN (Print): 1077-260X
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.139 SNIP 1.322 CiteScore 2.96
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.449 SNIP 1.393 CiteScore 3.03
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.889 SNIP 2.072 CiteScore 3.49
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.258 SNIP 2.38 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Investigation of CeO$_2$ Buffer Layer Effects on the Voltage Response of YBCO Transition-Edge Bolometers

The effect on the thermal parameters of superconducting transition-edge bolometers produced on a single crystalline SrTiO$_3$ (STO) substrate with and without a CeO$_2$ buffer layer was investigated. Metal-organic deposition was used to deposit the 20-nm CeO$_2$ buffer layer, whereas RF magnetron sputtering was applied to fabricate 150-nm-thick superconducting YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) thin film. The critical transition temperature for both of the YBCO films was 90 K, and the transition width was ~1.9 K. The bolometers fabricated from these samples were characterized with respect to the voltage phase and amplitude responses, and the results were compared with that of simulations conducted by applying a one-dimensional thermophysical model. It was observed that adding the buffer layer to the structure of the bolometer results in an increased response at higher modulation frequencies. Results from simulations made by fitting the thermal parameters in the model with and without an additional CeO$_2$ layer were found to be in agreement with the experimental observations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Sharif University of Technology
Authors: Mohajeri, R. (Ekstern), Nazifi, R. (Ekstern), Wulff, A. C. (Intern), Vesaghi, M. A. (Ekstern), Grivel, J. (Intern), Fardmanesh, M. (Ekstern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences
Investigation of CeO2.pdf
Investigation of the bonding strength and bonding mechanisms of SOFCs interconnector-electrode interfaces

General information
State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage, Applied Electrochemistry, Brno University of Technology, Academy of Sciences of the Czech Republic, Università degli Studi di Modena e Reggio Emilia
Authors: Boccaccini, D. N. (Intern), Sevecek, O. (Ekstern), Frandsen, H. L. (Intern), Dlouhy, I. (Ekstern), Molin, S. (Intern), Cannio, M. (Ekstern), Hjelm, J. (Intern), Hendriksen, P. V. (Intern)
Pages: 250–253
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 162
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.757 SNIP 0.935
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.792 SNIP 1.021 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 1.315 CiteScore 2.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.83 SNIP 1.237 CiteScore 2.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.924 SNIP 1.404 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.017 SNIP 1.568 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.059 SNIP 1.29
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.043 SNIP 1.276
BFI (2008): BFI-level 1
To enhance the Jc of YBa2Cu3O7−X (YBCO) films both in self-field and under magnetic field, an effective strategy is to introduce artificial pinning centers and keep a good YBCO matrix at the same time. Here, we propose a new dopant: LaAlO3 (LAO), based on its chemical stability and small mismatch toward YBCO. A series of YBCO films with different LAO doping contents was fabricated on LAO single-crystal substrates by metal organic deposition. We observed by X-ray diffractometer measurements and scanning electron microscopy observations that although a large amount of LAO is added, YBCO still keeps a good epitaxial growth relationship with LAO. Compared with a pure YBCO film, the Jc value of a 5.0% LAO-doped sample is enhanced more than three times in self-field 77 K and seven times at 77 K and 1.5 T, respectively. These results indicate that LAO doping can effectively enhance the Jc of YBCO films both in self-field and in applied magnetic fields.

**General information**

State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage
Authors: Xu, Y. (Ekstern), Suo, H. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern), Liu, M. (Ekstern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
Article number: 6602804
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
Joining of ceramic $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_3$ membranes for oxygen production to high temperature alloys

The possibility of joining dense ceramic BCSF tubular membranes to metal alloys using a silver braze was investigated. Four different alloys (Crofer 22 APU (R), Kanthal APM (R), Haynes 214 (R) and EN 1.4841) were considered and the influence of their oxide scale stability/reactivity and their thermal expansion coefficient on the stability of the final joint was evaluated. Leak tight assemblies were obtained only for steels with a thermal expansion coefficient of $> 16 \times 10^{-6} \text{K}^{-1}$ and protective coating. Proof-of-concept oxygen flux measurements up to 830 degrees C were performed on these assemblies, demonstrating the functionality of the developed hot sealing. In addition a simulation of the stresses occurring in the joint assembly during use was performed for different materials and geometries. The obtained results fit well with the experimental findings. (C) 2016 Elsevier B.V. All rights reserved.
Kinetic Studies on State of the Art Solid Oxide Cells: A Comparison between Hydrogen/Steam and Reformate Fuels

Electrochemical reaction kinetics at the electrodes of Solid Oxide Cells (SOCs) were investigated at 700 °C for two cells with different fuel electrode microstructures as well as on a third cell with a reduced active electrode area. Three fuel mixtures were investigated – hydrogen/steam and reformate fuels hydrogen/carbon-dioxide and hydrogen/methane/steam. It was found that the kinetics at the fuel electrode were exactly the same in both reformates. The hydrogen/steam fuel displayed slightly faster kinetics than the reformate fuels. Furthermore the gas conversion impedance in the hydrogen/steam fuel split into two processes with opposing temperature behavior in the reformate fuels. An 87.5 % reduction in active electrode area diminishes the gas conversion impedance in the hydrogen/steam fuel at high fuel flow rates. In both reformates, the second and third lowest frequency processes merged into a single process as the gas conversion was reduced. The SOC with finer electrode microstructure displayed improved kinetics.

General information
State: Published
Organisations: Applied Electrochemistry, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Karlsruher Institut für Technologie
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Number of pages: 12
Pages: F1451-F1462
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Journal
Volume: 163
Issue number: 13
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
A kinetic study of the chemical vapor deposition of tantalum in long narrow channels is done to optimize the industrial process for the manufacture of tantalum coated plate heat exchangers. The developed model fits well at temperatures between 750 and 850 °C, and in the pressure range of 25–990 mbar. According to the model, the predominant tantalum growth species is TaCl3. The temperature is shown to have a pronounced effect on the morphology and rate of deposition of the tantalum and an apparent change in deposition mechanism occurs between 850–900 °C, resulting in the deposition rate at 900 °C being lower than both 850 and 950 °C.
Large CZTS Nanoparticles Synthesized by Hot-injection for Thin Film Solar Cells

General information
State: Published
Organisations: Department of Photonics Engineering, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Optical Microsensors and Micromaterials, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Mirbagheri, N. (Intern), Simonsen, S. B. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Publication date: 2016
Event: Abstract from 2016 E-MRS Spring Meeting and Exhibit, Lille, France.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Laser beam induced current mapping (LBIG) of solar cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Jørgensen, M. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/gH4vyC-CUsg

Bibliographical note
Invited talk
Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2016
Lifetime of Nano-Structured Black Silicon for Photovoltaic Applications

In this work, we present recent results of lifetime optimization for nanostructured black silicon and its photovoltaic applications. Black silicon nano-structures provide significant reduction of silicon surface reflection due to highly corrugated nanostructures with excellent light trapping properties. We applied reactive ion etching technology at -20ºC to create nano-structures on silicon samples and obtained an average reflectance below 0.5%. For passivation purposes, we used 37 nm ALD Al2O3 films. Lifetime measurements resulted in 1220 µs and to 4170 µs for p- and n-type CZ silicon wafers, respectively. This is promising for use of black silicon RIE nano-structuring in a solar cell process flow.
Link between intermittent electrical energy sources and district heating sector
Energy has always been one of the key challenges in planning of societies' development worldwide. The COP conference in Paris in December 2015 has shown unprecedented mutual understanding of harmful consequences climate change can cause. Integrating power and heating sectors in an efficient way is an important step towards achieving the goals of the agreement in a cost-efficient way.
Localized Carbon Deposition in Solid Oxide Electrolysis Cells Studied By Multiphysics Modeling

Modeling for optimizing performance has attracted substantial research efforts in the last twenty years with special focus on solid oxide fuel cells (SOFCs). However, limited amount of the modeling work has been focused on the solid oxide electrolysis cell (SOEC) operation mode and even less on degradation issues connected to SOEC operation. Despite the similarities between the two operation modes, the different operating voltage ranges and the gradients involved influence the long-term degradation and performance in different ways.

Long-term operation of a solid oxide cell stack for coelectrolysis of steam and CO2

High temperature electrolysis based on solid oxide electrolysis cells (SOECs) is a promising technology for production of synthetic fuels. The SOEC units can be used for co-electrolysis of steam and CO2 to produce synthesis gas (syngas, CO+H2), which can be further processed to a variety of synthetic fuels such as methane, methanol or DME. Previously we have reported electrolysis operation of solid oxide cell stacks for periods up to about 1000 hours. In this work, operation of a Haldor Topsoe 8-cell stack (stack design of 2014) in co-electrolysis mode for 6000 hours is reported. The stack consists of Ni/YSZ electrode supported SOEC cells with a footprint of 12X12 cm2. The co-electrolysis operation was carried out by supplying a mixture of 45 % CO2 + 45 % H2O + 10 % H2 to the stack operating with a fixed conversion of 39 % for steam and CO2. The stack was operated at different conditions. Initial operation at 700 oC and -0.25 A/cm2 lasted for only 120 hours due to severe degradation of the bottom cell. Regaining the stack performance was realized by increasing the operation temperature to 750 oC. After reactivation, the stack showed negligible degradation at 750 oC and -0.25 A/cm2 and about 1.4 %/1000 h performance degradation at 750 oC and -0.5 A/cm2. This study demonstrates feasibility of long-term co-electrolysis operation via SOEC stacks and of careful temperature variation as a tool to regain the stack performance.
Long-Term Stability of Anode-Supported Solid Oxide Fuel Cells with a Co-Sintered Cathode Backbone and Infiltrated La$_{0.95}$Co$_{0.4}$Ni$_{0.6}$O$_3$ (LCN) Electro-Catalyst

Infiltration is a fabrication method that is offering potentially significant improvements in cell performance at reduced materials and fabrication costs, especially when combined with co-sintering. However, important questions regarding the long-term performance and microstructural stability of infiltrated electrodes, as well as the mechanical properties of such electrodes have remained unanswered.

**General information**
- **State:** Published
- **Organisations:** Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors, Imaging and Structural Analysis, Haldor Topsoe AS
- **Authors:** Küngas, R. (Ekstern), Veltzé, S. (Intern), Ovtar, S. (Intern), Xu, Y. (Intern), Simonsen, S. B. (Intern), Kwok, K. (Intern), Frandsen, H. L. (Intern), Samson, A. J. (Intern), Zielke, P. (Intern), Kiebach, W. (Intern)
- **Conference:** PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Electrochemical Society. Meeting Abstracts (Online)
- **Volume:** MA2016-02
- **Article number:** 2895
- **ISSN (Print):** 2151-2043
- **Original language:** English
- **Links:** http://ma.ecsdl.org/content/MA2016-02/39/2895.abstract?sid=4e5162bc-0faa-4dfe-9995-942c35cb5b43
- **Publication:** Research - peer-review › Conference abstract in journal – Annual report year: 2016

Low cost porous MgO substrates for oxygen transport membranes

This paper delineates the fabrication of porous magnesium oxide (MgO) ceramics with high porosity and gas permeability by warm pressing using pre-calcined MgO powder and fugitive pore former (combination of graphite and polymethyl methacrylate). Effect of pore former on the microstructure development of porous MgO ceramic substrates was subjected to investigation. The resultant microstructure consisted of large spherical and elongated pores with small interconnecting pores. The total porosity (55%), mean pore neck size (0.65 μm), and the associated gas permeability (4–4.5×10⁻¹⁵ m²) of MgO substrates were measured and correlated. Economic analysis of the MgO substrates was performed and it was found that MgO was much cheaper compared to perovskite and fluorite materials.

**General information**
- **State:** Published
- **Organisations:** Department of Energy Conversion and Storage, Swiss Federal Laboratories for Materials Science and Technology (Empa)
- **Authors:** Kothanda Ramachandran, D. (Intern), Søgaard, M. (Intern), Clemens, F. (Ekstern), Sudireddy, B. R. (Intern), Kaiser, A. (Intern)
- **Number of pages:** 3
- **Pages:** 254-256
- **Publication date:** 2016
Porous MgO ceramics, Gas permeability, Membrane, Low cost supports, Thermoplastic system

DOI: 10.1016/j.matlet.2016.01.142
Source: FindIt
Source-ID: 2291745807
Publication: Research - peer-review › Journal article – Annual report year: 2016
Low temperature processed MnCo$_2$O$_4$ and MnCo$_{1.8}$Fe$_{0.2}$O$_4$ as effective protective coatings for solid oxide fuel cell interconnects at 750 °C

In this study two materials, MnCo2O4 and MnCo1.8Fe0.2O4 are studied as potential protective coatings for Solid Oxide Fuel Cell interconnects working at 750 °C. First powder fabrication by a modified Pechini method is described followed by a description of the coating procedure. The protective action of the coating applied on Crofer 22 APU is evaluated by following the area specific resistance (ASR) of the scale/coating for 5500 h including several thermal cycles. The coating is prepared by brush painting and has a porous structure after deposition. Post mortem microstructural characterization performed on the coated samples shows good protection against chromium diffusion from the chromia scale ensured by a formation of a dense reaction layer. This study shows, that even without high temperature sintering and/or reactive sintering it is possible to fabricate protective coatings based on MnCo spinels.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology, Jilin University
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Number of pages: 11
Pages: 408-418
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 336
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
LSCF fibers for IT-SOFCs applications: synthesis and morphological analysis

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, University of Genoa
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Number of pages: 1
Publication date: 2016
Event: Abstract from ELectrospinning for ENergy Conference, Montpellier, France.
Main Research Area: Technical/natural sciences
Electronic versions:
elen2016_EnricoAnna_vers.1.pdf
Publication: Research › Conference abstract for conference – Annual report year: 2016

Magnetocaloric materials and first order phase transitions
This thesis studies the first order phase transitions of the magnetocaloric materials La_{0.67}Ca_{0.33}MnO_3 and La(Fe,Mn,Si)_{13}H_x trying to overcome challenges that these materials face when applied in active magnetic regenerators. The study is done through experimental characterization and modelling of the properties of such materials. The experimental characterization of these materials is done through various different methods, such as X-ray diffraction, magnetometry, calorimetry, direct measurements of entropy change, capacitance dilatometry, scanning electron microscopy, energy-dispersive X-ray spectrometry and magnetocaloric regenerative tests. The magnetic, thermal and structural properties obtained from such measurements are then evaluated through different models, i.e. the Curie-Weiss law, the Bean-Rodbell model, the free electron model and the Debye model. The measured magnetocaloric properties of La_{0.67}Ca_{0.33}MnO_3 shows a paradoxical behavior; the material shows features of both a first order phase transition and of a second order one. Identities as shift of the heat capacity peak and an asymmetric growth of of the entropy change with magnetic field would describe this material transition as a first order one. However, the material did not present any signs of intrinsic hysteresis, a feature common in first order transitions. This is attributed to a chemical distribution in this first order phase transition material that can lead to a smearing of the transition and the hysteresis, and such effect is observed through modelling. Moreover, inverse susceptibility measurements showed what could be evidences of magnetic polarons being formed in the paramagnetic phase of the material. The origin of the first order transition seems to be due to the magneto-elastic coupling observed through isothermal magnetstriction and dilatometric measurements. Although the Bean-Rodbell model has described with a good agreement the entropy change, hysteresis, magnetization and heat capacity, it has failed to describe the isothermal magnetstriction. It is suggested that such failure could be related to different factors that might
The Bean-Rodbell model describes the second order magnetic phase transition in materials like La(Fe,Mn,Si)$_{13}H_y$ with first order phase transition. The model assumes that for a fixed magnetic field, the material undergoes a second order transition for $\eta > 1$, while for $\eta \leq 1$ it undergoes a first order transition. 

The magnetic interactions in these materials are such that the magnetic field depends on the unit cell volume. This coupling is defined by the model parameter $\eta$, where for $\eta = 1$ the material undergoes a second order transition, and for $\eta < 1$ a first order transition. The transition temperature can be controlled through the Mn and Si content, which influences the magnetic interactions.

However, the model over-predicts the thermal hysteresis and under-predicts the shift of the transition temperature with temperature. The model describes with good agreement the volume discontinuity across the phase transition, and the model is applied to describe the volumetric behavior observed through X-ray measurements as a function of the transition. After this effect, if the entropy change is remeasured it shows very similar behavior to measurements of ground particles. Therefore, the results suggest that defects inserted through grinding is probably not the case. To explain such behavior, in this thesis it is proposed that slightly differences in the composition throughout the sample may lead to a Curie temperature distribution. This in turn would lead to different regions of the sample undergoing the transition in different temperatures. However, given the polycrystallinity of the material, the crystallites with different Curie temperatures will be volumetrically constrained until enough energy is given to the system and the whole bulky particle undergoes the transition. This explains why bulky particles have a sharp transition, while ground particles have a smoother one; the latter is much less volumetrically constrained than the former. An outcome of such behavior is observed as strain development through the transition. This strain was calculated applying the Williamson-Hall method. The strain development is much more significant in the ferromagnetic phase than in the paramagnetic one, which is attributed to the weakening of the magnetic interactions as the ferromagnetic phase approaches the transition. This is speculated as a decrease of the bulk modulus of the ferromagnetic phase as the temperature increases. The paramagnetic phase, however, is expected to have a relatively constant bulk modulus as there is no magnetic interactions. When observing the microscopy images, they show that cracks are usually somehow connected to the brittle and hard phase that does not present a volume change. Therefore, the decrease of this phase, however low content it is, could lead to an improvement in the mechanical stability of the material during application. Finally, the Bean-Rodbell model is applied to describe the volumetric behavior observed through X-ray measurements as a function of the temperature. The model describes with good agreement the volume discontinuity across the phase transition, and the superimposed distribution of Curie temperature can describe well the paramagnetic growth as the transition occurs.

However, the model over-predicts the thermal hysteresis and under-predicts the shift of the transition temperature with magnetic field.
distribution of the transition temperature with a standard deviation $\sigma_T$, in order to model the chemical inhomogeneity. Good agreement is obtained between measurements and model with values of $\eta \sim 1.8$ and $\sigma(T) = 1.0$ K.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Atomic scale modelling and materials  
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Norby, P. (Intern), Smith, A. (Intern), Bahl, C. R. H. (Intern)  
Number of pages: 7  
Publication date: 2016  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: A I P Advances  
Volume: 6  
Issue number: 5  
Article number: 056217  
ISSN (Print): 2158-3226  
Ratings:  
Web of Science (2017): Indexed Yes  
Scopus rating (2016): CiteScore 1.32 SJR 0.449 SNIP 0.612  
Web of Science (2016): Indexed yes  
Scopus rating (2015): SJR 0.457 SNIP 0.619 CiteScore 1.17  
Web of Science (2015): Indexed yes  
Scopus rating (2014): SJR 0.709 SNIP 0.788 CiteScore 1.38  
Web of Science (2014): Indexed yes  
Scopus rating (2013): SJR 0.769 SNIP 0.906 CiteScore 1.36  
ISI indexed (2013): ISI indexed yes  
Scopus rating (2012): SJR 0.822 SNIP 0.897 CiteScore 1.14  
ISI indexed (2012): ISI indexed no  
Web of Science (2011): Indexed yes  
Original language: English  
Electronic versions: Magneto_elastic_coupling.pdf  
DOIs: 10.1063/1.4944400

**Bibliographical note**

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Source: FindIt  
Source-ID: 277373393  
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Manufacture, installation and decommissioning of organic solar cell parks**

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials  
Authors: Søndergaard, R. R. (Intern)  
Publication date: 2016

**Publication information**

Media of output: Video  
Original language: English  
Publisher: DTU Energy  
Main Research Area: Technical/natural sciences  
Links: https://youtu.be/JMcAN88OeQs

**Bibliographical note**

Invited talk
Manufacturing of a LaNiO$_3$ composite electrode for oxygen evolution in commercial alkaline water electrolysis

The LaNiO$_3$ perovskite was chosen for incorporation into a nickel matrix in order to obtain a metallic composite electrode suitable for improving the oxygen evolution reaction (OER) in commercial water electrolysis at elevated temperature. The manufactured LaNiO$_3$ + Ni composite coatings were deposited in a Watts type nickel electrolyte in a specially designed beaker with continuous particle circulation. Activity of the composite coatings was evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and anodic potentiodynamic polarization measurements. The obtained results were compared to a non-catalysed Watts nickel reference sample and the electrochemical measurements confirmed that the coating decreased the OER overpotential by 70 mV. XRD furthermore revealed that a LaNiO$_3$ + Ni composite structure was obtained. Conventional alkaline water electrolysis was carried out at a temperature of 120 °C and a current densities of 0.2 and 0.8 A cm$^{-2}$. Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS) and X-ray Diffraction (XRD) were used for characterization of the morphology.
Electricity consumption is often the hotspot of life cycle assessment (LCA) of products, industrial activities, or services. The objective of this paper is to provide a consistent, scientific, region-specific electricity-supply-based inventory of electricity generation technology for national and regional power grids. Marginal electricity generation technology is pivotal in assessing impacts related to additional consumption of electricity. China covers a large geographical area with regional supply grids; these are arguably equally or less integrated. Meanwhile, it is also a country with internal imbalances in regional energy supply and demand. Therefore, we suggest an approach to achieve a geographical subdivision of the Chinese electricity grid, corresponding to the interprovincial regional power grids, namely the North, the Northeast, the East, the Central, the Northwest, and the Southwest China Grids, and the China Southern Power Grid. The approach combines information from the Chinese national plans on for capacity changes in both production and distribution grids, and knowledge of resource availability. The results show that nationally, marginal technology is coal-fired electricity generation, which is the same scenario in the North and Northwest China Grid. In the Northeast, East, and Central China Grid, nuclear power gradually replaces coal-fired electricity and becomes the marginal technology. In the Southwest China Grid and the China Southern Power Grid, the marginal electricity is hydropower towards 2030.
Due to the ever growing demand for sustainable energy alternatives, increasing the efficiency as well as reliability of energy conversion and storage technologies is becoming paramount challenge for the research community in the field. To achieve this, the innovation of new material systems should go hand in hand with understanding and improving their mechanical reliability at operational conditions. With this regard, DTU energy has a dedicated team and facilities working on characterization of metallic as well as ceramic materials used in energy conversion and storage technologies. The poster presents the unique capabilities in the department including high throughput and high temperature strength and deformational behavior characterization of materials in a controlled atmosphere. The characterization techniques mainly focus on materials being developed to be used in solid oxide fuel or electrolysis cells, oxygen or gas membranes, etc.
Mechanical Properties of a Library of Low-Band-Gap Polymers

The mechanical properties of low-band-gap polymers are important for the long-term survivability of roll to roll processed organic electronic devices. Such devices, e.g., solar cells, displays, and thin-film transistors, must survive the rigors of roll-to-roll coating and also thermal and mechanical forces in the outdoor environment and in stretchable and ultraflexible form factors. This paper measures the stiffness (tensile modulus), ductility (crack-onset strain), or both of a combinatorial library of 51 low-band-gap polymers. The purpose of this study is to systematically screen a library of low-band-gap polymers to better understand the connection between molecular structures and mechanical properties in order to design conjugated polymers that permit mechanical robustness and even extreme deformability. While one of the principal conclusions of these experiments is that the structure of an isolated molecule only partially determines the mechanical properties another important codeterminant is the packing structure some general trends can be identified. (1) Fused rings tend to increase the modulus and decrease the ductility. (2) Branched side chains have the opposite effect. Despite the rigidity of the molecular structure, the most deformable films can be surprisingly compliant (modulus >= 150 MPa) and ductile (crack-onset strain).
Mg/O2 Battery Based on the Magnesium-Aluminum Chloride Complex (MACC) Electrolyte

MgO2 cells employing a MgCl2/AlCl3/DME (MACC/DME) electrolyte are cycled and compared to cells with modified Grignard electrolytes, showing that performance of magnesium/oxygen batteries depends strongly on electrolyte composition. Discharge capacity is far greater for MACC/DME-based cells, while rechargeability in these systems is severely limited. The MgO2-MACC/DME discharge product comprises a mixture of Mg(ClO4)2 and MgCl2, with the latter likely formed from slow decomposition of the former. The presence of Cl in these compounds suggests that the electrolyte participates in the cell reaction or reacts readily with the initial electrochemical products. A rate study suggests that O2 diffusion in the electrolyte limits discharge capacities at higher currents. Formation of an insulating product film on the positive electrodes of Mg/O2-MACC/DME cells following deep discharge increases cell impedance substantially and likely explains the poor rechargeability. An additional impedance rise consistent with film formation on the Mg negative electrode suggests the presence of detrimental O2 crossover. Minimizing O2 crossover and bypassing charge transfer through the discharge product would improve battery performance.

General information
State: Published
Organisations: Atomic scale modelling and materials, Department of Energy Conversion and Storage, University of Michigan, DENSO Corporation, DENSO International America, University of Oxford
Authors: Vardar, G. (Ekstern), Smith, J. G. (Ekstern), Thomson, T. (Ekstern), Inagaki, K. (Ekstern), Naruse, J. (Ekstern), Hiramatsu, H. (Ekstern), Sleightholme, A. E. S. (Ekstern), Sakamoto, J. (Ekstern), Siegel, D. J. (Intern), Monroe, C. W. (Ekstern)
Number of pages: 9
Pages: 7629-7637
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry of Materials
Volume: 28
Issue number: 21
ISSN (Print): 0897-4756
Ratings:
BFI (2018): BFI-level 2
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow

This thesis presents numerical modeling of active magnetic regenerator (AMR) and passive regenerator tests with oscillating flow. The work serves to investigate and improve the understanding of emerging concepts and technologies in the area of magnetic refrigeration. The discretization scheme of a one dimensional (1D) AMR model is improved for decreasing spurious temperature oscillations in the numerical solution. This transient AMR model is further modified for simulating tapered regenerators, heat loss through the housing wall and regenerators using mixed materials. Magnetocaloric materials (MCM) with a first or second order phase transition (FOPT or SOPT) exhibit different characteristics in isothermal entropy change $\Delta S_{iso}$, adiabatic temperature change $\Delta T_{ad}$ and temperature dependence of the magnetocaloric effect (MCE). A theoretical study quantifies the impact of these parameters, showing that all of them are equally important. Based on measured magnetocaloric properties of La(Fe,Mn,Si)$_{13}H_y$ and Gd, a thorough investigation on how to layer typical FOPT or SOPT materials is implemented. For those regenerators, the sensitivity to the working temperature and the Curie temperature variation is evaluated. A concept of mixing FOPT and SOPT materials is also investigated. Furthermore, the entropy production rates due to insufficient heat transfer, viscous dissipation and axial conduction, as well as the total entropy production rate, are calculated and compared for analyzing different loss mechanisms and optimizing AMRs. The impacts of the heat loss through the regenerator housing and the dead volume are also quantified. A multiparameter optimization reveals the optimal dimensions and operating parameters for different regenerator geometries. In order to evaluate different regenerator geometries, including the emerging epoxy bonded bed and different heat transfer fluids, a passive regenerator test apparatus is constructed and an experimental investigation is presented. The flow and heat transfer characteristics of different regenerators are estimated by presenting the measured and deduced indicators, including the pressure drop, friction factor, effectiveness, heating power and overall Nusselt number. Finally, based on the research in this thesis, the perspectives and some suggestions for the future work are given.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Syddansk Universitet
Authors: Lei, T. (Intern), Engelbrecht, K. (Intern), Nielsen, K. K. (Intern), Veje, C. T. (Ekstern)
Number of pages: 270
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Modeling_of_active_magnetic_regenerators.pdf

Relations
Projects:
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow
Publication: Research › Ph.D. thesis – Annual report year: 2016

Modeling of transport phenomena in battery cathode materials

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Technical University of Denmark
Authors: García Lastra, J. M. (Intern), Mekonnen, Y. S. (Intern), Loftager, S. (Intern), Melander, M. (Intern), Mathiesen, N. R. (Ekstern), Christensen, R. (Intern), Vegge, T. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
ABSTRACT_Garcia_Lastra_The_Hague.pdf
Source: PublicationPreSubmission
Source-ID: 128083393
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Modelling transition towards sustainable transportation sector
Modelling Transition Towards Sustainable Transportation Sector

In a transition towards 100% renewable energy system, transportation sector is rarely dealt with using the holistic approach and measuring its impact on the whole energy system. Furthermore, solutions for power and heat sectors are clearer, it is a tendency of the researchers to focus on the latter two energy sectors. In order to deal with the raised issue, authors of this paper developed a methodology for calculation of the transition towards sustainable transport sector, focusing on the solutions that are already available. Furthermore, as a part of the model, a detailed mapping of resources needed has been carried out for each of the alternatives. It was shown that the electrification of the transportation sector is a crucial point in transition, while for the transport modes that cannot be electrified, or shifted to different transportation modes, four alternatives were defined: synthetic fuels, biofuels, hydrogen and synthetic fuels utilizing excess intermittent electricity generation. Results showed that the 72.3% of the fossil fuel demand in transportation sector of the European Union (EU) can be replaced by electricity demand, reducing final energy demand in transportation sector for 50.6% or 2,051 TWh. All the alternatives for the non-electrified part of transportation suffer from the low well-to-wheel efficiency, resulting in a significant amount of additional resources needed. Replacing remaining part of the fossil fuels by biofuels led to the increased demand for biomass on EU level equal to 3,069 TWh, which is extremely challenging to meet in the future in a sustainable way. In the case of synthetic fuel production as an alternative, additional electricity demand was calculated to be 2,775 TWh, which is approximately 90% of the total electricity demand of the EU for the year 2013. Hence, authors argued that due to the enormous additional demand for scarce resources for producing alternatives to the fossil fuels, concepts such as car sharing, induction charging on highways, promotion of bicycling and public transportation should be assessed in more detailed way in order to bring additional energy savings in the sector.

Molecular dynamics simulations of ternary Pt_xPd_yAu_z fuel cell nanocatalyst growth

Molecular dynamics simulation of PEMFC cathodes based on ternary Pt_{70}Pd_{15}Au_{15} and Pt_{50}Pd_{25}Au_{25} nanocatalysts dispersed on carbon indicate systematic Au segregation from the particle bulk to the surface, leading to an Au layer coating the cluster surface and to the spontaneous formation of a Pt@Pd@Au core-shell structure. For Au content below 25 at%, surface Pt_{Pd} active sites are available for efficient oxygen reduction reaction, in agreement with DFT calculations and experimental data. Simulations of direct core@shell system prepared in conditions mimicking those of plasma sputtering deposition pointed out an increase of the number of accessible Pt_{Pd} surface active sites. Core-shell nanocatalyst morphology changes occur due to impinging Pt kinetic energy confinement and dissipation.
Nanocomposite YSZ-NiO Particles with Tailored Structure Synthesized in a Two-Stage Continuous Hydrothermal Flow Reactor

The increasing amount of fluctuating electricity generation from renewable sources requires a flexible energy system and storage technologies to ensure that energy services can be covered in a stable and affordable manner. In order to become truly independent from fossil fuels, increasing the performance of energy storage and conversion devices such as fuel cells, electrolyzers and batteries is important. One promising approach to further improve these devices is the use of carefully structured nanosized materials. Nano-composite particles combining different materials in advanced geometries like core-shell structures or surface decorated particles could exhibit better performance compared with single phase materials. To obtain such advanced structures is the aim of the ProEco project (www.proeco.dk). In this project, a two-stage continuous reactor is built and used to synthesize such nano-composites.

Here we report on the design of the two-stage continuous hydrothermal flow synthesis reactor and first results on obtaining structured nano-composite consisting of yttria-stabilized zirconia (YSZ) and NiO materials. These materials are commonly applied in the fuel electrodes of today’s state-of-the-art solid oxide fuel and electrolysis cells. The prepared particles were characterized by X-ray powder diffraction, (high resolution) transmission electron microscopy, scanning tunnel transmission microscopy and Raman spectroscopy in order to determine crystal structure, particle size, surface morphology and element distribution.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Atomic scale modelling and materials
Authors: Zielke, P. (Intern), Xu, Y. (Intern), Kiebach, W. (Intern), Simonsen, S. B. (Intern), Norby, P. (Intern), Hendriksen, P. V. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2953
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/39/2953
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2016

Nanocoentrainment of LiBH₄ for High Ionic Conductivity in Lithium Ion Batteries

Efficient energy conversion and storage is crucial for development of systems based on renewable energy sources. For electricity storage, Li-ion batteries are commonly used in electronics devices but require many improvements to obtain longer life-time and higher energy densities. The current use of organic liquids and gels electrolytes limits these improvements because of lithium dendrites formation, reducing the lifetime of the battery and which can possibly be hazardous due to risks of short circuits.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Nanostructured materials for solid-state hydrogen storage: A review of the achievement of COST Action MP1103

In the framework of the European Cooperation in Science and Technology (COST) Action MP1103 Nanostructured Materials for Solid-State Hydrogen Storage were synthesized, characterized and modeled. This Action dealt with the state of the art of energy storage and set up a competitive and coordinated network capable to define new and unexplored ways for Solid State Hydrogen Storage by innovative and interdisciplinary research within the European Research Area. An important number of new compounds have been synthesized: metal hydrides, complex hydrides, metal halide ammines and amidoboranes. Tuning the structure from bulk to thin film, nanoparticles and nanococonfined composites improved the hydrogen sorption properties and opened the perspective to new technological applications. Direct imaging of the hydrogenation reactions and in situ measurements under operando conditions have been carried out in these studies. Computational screening methods allowed the prediction of suitable compounds for hydrogen storage and the modeling of the hydrogen sorption reactions on mono-, bi-, and three-dimensional systems. This manuscript presents a review of the main achievements of this Action. © 2016 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.
New Hypothesis for SOFC Ceramic Oxygen Electrode Mechanisms

A new hypothesis for the electrochemical reaction mechanism in solid oxide cell ceramic oxygen electrodes is proposed based on literature including our own results. The hypothesis postulates that the observed thin layers of SrO-La$_2$O$_3$ on top of ceramic perovskite and other Ruddlesden-Popper structured electrode materials are sufficiently electron and oxygen ion conducting to provide reaction sites despite that the bulk phase of such an oxide layer is insulating. We claim that a few
A nanometer thin layer of mixed SrO-La$_2$O$_3$ that contains some dissolved transition metal and some impurities plus two space charge layers – one towards the gas phase and the other towards the perovskite – will be sufficiently oxide ion (vacancy) and electron conducting to support the electrode process. We also present some considerations about a possible mechanism of improved electrodes.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Imaging and Structural Analysis
Number of pages: 11
Pages: 93-103
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: ECS Transactions
Volume: 72
Issue number: 7
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
DOIs:
10.1149/07207.0093ecst
Source: PublicationPreSubmission
Source-ID: 123882757
Publication: Research - peer-review › Conference article – Annual report year: 2016

**New Insights into the Creation of High-Mobility Two-Dimensional Electron Gas at Oxide Interfaces: Control of Interfacial Redox Reactions by an Electron Sink**

**General information**
Ni/YSZ electrodes structures optimized for increased electrolysis performance and durability

Cermet Ni/YSZ electrodes are the most commonly applied fuel electrode for solid oxide cells (SOC) both when targeting solid oxide fuel cell (SOFC) applications and when used as solid oxide electrolysis cell (SOEC). In this work we report on the correlation between initial Ni/YSZ microstructure and the resulting electrochemical performance both initially and during long-term electrolysis testing at high current density and high p(H₂O) inlet. Especially, this work focuses on microstructure optimization to hinder Ni mobility and migration during long-term operation and illustrates the key-role of electrode over-potential on the degradation of the Ni/YSZ electrodes in SOEC. We find that for long-term stability for electrolysis at high current densities and high p(H₂O) the as-produced NiO/YSZ precursor electrode should be: 1) As dense as possible, 2) as fine particle and pore sized as possible and 3) the three phases (Ni, YSZ and pore phase) shall be size-matched and well-dispersed. Applying such microstructure, optimized Ni/YSZ electrode we show SOEC test results with long-term degradation rate as low as 0.3-0.4%/kh at -1 A/cm², 800 °C and inlet gas mixture of p(H₂O)/p(H₂):90/10. This enables SOEC operation of such cell for more than 5 years below thermo-neutral potential at these operating conditions.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Mixed Conductors, Fundamental Electrochemistry
Authors: Hauch, A. (Intern), Brodersen, K. (Intern), Chen, M. (Intern), Mogensen, M. B. (Intern)
Number of pages: 10
Pages: 27-36
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 293
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Non-Platinum Oxygen Reduction Catalysts. From Crystalline to Molecular Moieties

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 4th International Workshop on Solution Plasma and Molecular Technology (SPM-4), Pilsen, Czech Republic.
Main Research Area: Technical/natural sciences

Bibliographical note
Invited talk
Source: PublicationPreSubmission
Nonuniversal scaling of the magnetocaloric effect as an insight into spin-lattice interactions in manganites

We measure the magnetocaloric effect of the manganite series La0.67Ca0.33-xSrxMnO3 by determining the isothermal entropy change upon magnetization, using variable-field calorimetry. The results demonstrate that the field dependence of the magnetocaloric effect close to the critical temperature is not given uniquely by the critical exponents of the ferromagnetic-paramagnetic phase transition, i.e., the scaling is nonuniversal. A theoretical description based on the Bean-Rodbell model and taking into account compositional inhomogeneities is shown to be able to account for the observed field dependence. In this way the determination of the nonuniversal field dependence of the magnetocaloric effect close to a phase transition can be used as a method to gain insight into the strength of the spin-lattice interactions of magnetic materials. The approach is shown also to be applicable to first-order transitions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Secretariat, IT, Electrofunctional materials
Authors: Smith, A. (Intern), Nielsen, K. K. (Intern), Neves Bez, H. (Intern), Bahl, C. (Intern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B
Volume: 94
Issue number: 5
Article number: 054411
ISSN (Print): 2469-9950
Ratings:
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.982 SNIP 1.524
Novel ceramic processing method for substitution of toxic plasticizers

A systematic screening of plasticisers for a polyvinyl butyral based binder system revealed that dibutyl maleate, dibutyl adipate and Pycal 94 are promising and less toxic alternatives to the very harmful but frequently used dibutyl phthalate. Pycal 94 seems especially promising as it unlike the two other candidates did not require a co-plasticiser, such as a polyethylene glycol, thus simplifying the system and reducing the risk of unwanted cross-interactions. An effective and systematic procedure for substitution of the plasticiser, while maintaining chemical compatibility and mechanical properties, was also demonstrated. Incompatible systems were discarded in an initial broad screening while primary systems were further evaluated based on debinding properties, mechanical properties, flow behavior as well as sintering properties of ceramic tapes. The thermomechanical characterization performed on dried drops of binder and their corresponding tapes show strong similarities in the strain/stress profiles, validating the qualitative method used.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Foghmoes, S. P. V. (Intern), Teocoli, F. (Intern), Brodersen, K. (Intern), Klemensø, T. (Intern), Della Negra, M. (Intern)
Number of pages: 9
Pages: 3441-3449
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 36
Issue number: 14
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Novel high band gap pendant-borylated carbazole polymers with deep HOMO levels through direct $^+$N=$^-$B$^-$ interaction for organic photovoltaics

In this communication, we investigate the direct and still conjugated intramolecular $^+$N=$^-$B$^-$ interactions in novel high band gap borylated carbazole containing polymers, namely, poly(3,6-(N-di(2,4,6-trimethyl)-phenylboryl-carbazole)-alt- 4,8-di(5-(2-ethylhexyl)thiophene-2-yl)benzo[1,2-b: 4,5-b'] dithiophene) (P(3,6-BCBDT)) and poly(3,6-(N-di(2,4,6-trimethyl)phenylboryl-carbazole)-alt-3,3 "'-didodecyl-2,2'; 5',2'; 5"',2"'-quaterthiophene) (P(3,6-BCQT)), which result in ambipolarity, high electron affinity, and deep HOMO levels. The quasi-donor-acceptor nature of the two polymers was confirmed by UV-Vis absorption, electro-chemical property studies, and computer modelling. Band gaps of 2.07 eV for
P(3,6-BCBDT) and 2.23 eV for P(3,6-BCQT) were obtained. P(3,6-BCQT) afforded a power conversion efficiency of 1.44%, with a J_sc of 4.82 mA cm^{-2}, a V_oc of 0.79 V and a FF of 37%, and P(3,6-BCBDT) performed better with an efficiency of 3.82%, with a J_sc of 8.31 mA cm^{-2}, a V_occ of 1.0 V based on its low lying HOMO level, and a FF of 45%.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Aalborg University, Chinese Academy of Sciences
Number of pages: 9
Pages: 4393-4401
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Materials Chemistry C
Volume: 4
Issue number: 20
ISSN (Print): 2050-7526
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.14 SJR 1.806 SNIP 1.28
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.751 SNIP 1.577 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.505 SNIP 1.36 CiteScore 4.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Original language: English
DOIs:
10.1039/c6tc01208f
Source: FindIt
Source-ID: 2303885778
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Novel micro-reactor flow cell for investigation of model catalysts using in situ grazing-incidence X-ray scattering**

The design, fabrication and performance of a novel and highly sensitive micro-reactor device for performing in situ grazing-incidence X-ray scattering experiments of model catalyst systems is presented. The design of the reaction chamber, etched in silicon on insulator (SIO), permits grazing-incidence small-angle X-ray scattering (GISAXS) in transmission through 10 µm-thick entrance and exit windows by using micro-focused beams. An additional thinning of the Pyrex glass reactor lid allows simultaneous acquisition of the grazing-incidence wide-angle X-ray scattering (GIWAXS). In situ experiments at synchrotron facilities are performed utilizing the micro-reactor and a designed transportable gas feed and analysis system. The feasibility of simultaneous in situ GISAXS/GIWAXS experiments in the novel micro-reactor flow cell was confirmed with CO oxidation over mass-selected Ru nanoparticles.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Individual Nanoparticle Functionality, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Experimental Surface and Nanomaterials Physics, Paul Scherrer Institut
Number of pages: 9
Pages: 455-463
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Synchrotron Radiation
Volume: 23
Issue number: 2
ISSN (Print): 0909-0495
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.593 SNIP 1.578
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.161 SNIP 1.396 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.505 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.473 SNIP 1.687 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.558 SNIP 1.273 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.503 SNIP 1.424 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.618 SNIP 1.479
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.496 SNIP 1.373
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.938 SNIP 1.637
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.8 SNIP 2.363
Scopus rating (2006): SJR 1.517 SNIP 1.149
Scopus rating (2005): SJR 1.254 SNIP 1.469
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.695 SNIP 0.74
Scopus rating (2003): SJR 0.624 SNIP 0.817
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.541 SNIP 0.573
Scopus rating (2001): SJR 1.132 SNIP 1.724
Scopus rating (2000): SJR 0.67 SNIP 0.747
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.829 SNIP 0.95
Original language: English
GISAXS, GIWAXS, in situ, micro-reactor
Electronic versions:
PESEI_fv5041.pdf
DOIs:
10.1107/S1600577516001387
On Degradation Issues in High-Temperature Electrochemical Devices

**General information**

State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Forschungs Zentrum Jülich GmbH
Authors: De Haart, L. (Ekstern), Holtappels, P. (Intern)
Number of pages: 37
Publication date: 2016

**Publication information**

Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:

On performance limitations and property correlations of Al-doped ZnO deposited by radio-frequency sputtering: Paper

The electrical properties of RF-sputtered Al-doped ZnO are often spatially inhomogeneous and strongly dependent on deposition parameters. In this work, we study the mechanisms that limit the minimum resistivity achievable under different deposition regimes. In a low- and intermediate-pressure regime, we find a generalized dependence of the electrical properties, grain size, texture, and Al content on compressive stress, regardless of sputtering pressure or position on the substrate. In a high-pressure regime, a porous microstructure limits the achievable resistivity and causes it to increase over time as well. The primary cause of inhomogeneity in the electrical properties is identified as energetic particle bombardment. Inhomogeneity in oxygen content is also observed, but its effect on the electrical properties is small and limited to the carrier mobility.

**General information**

State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Physics, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Crovetto, A. (Intern), Ottsen, T. S. (Ekstern), Stamate, E. (Intern), Kjær, D. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 11
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Volume: 49
Issue number: 29
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.645 SNIP 0.917
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.693 SNIP 1.046 CiteScore 2.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.069 SNIP 1.383 CiteScore 2.53
On the Challenges of Reducing Contact Resistances in Thermoelectric Generators Based on Half-Heusler Alloys

A method using fast hot pressing to join half-Heusler (HH) thermoelectric materials directly to an electrical current collector (Ag electrode) without using a third filler material is introduced. The compositions of the HH alloys used are Hf0.5Zr0.5CoSn0.2Sb0.8 and Ti0.6Hf0.4NiSn for p- and n-type, respectively. Using this method, the quality of the HH–electrode contacts is improved due to their low electrical contact resistance and less reaction–diffusion layer. The microstructure and chemical composition of the joints were examined using a scanning electron microscope equipped with energy dispersive x-ray analysis. The electrical characteristics of the interfaces at the contacts were studied based on
electrical contact resistance and Seebeck scanning microprobe measurements. In this paper, we show that joining the HH to a Ag electrode directly using fast hot pressing resulted in lower contact resistance and better performance compared with the method of using active brazing filler alloy.

**General information**

State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Aarhus University, Johannes Gutenberg University
Authors: Pham, H. N. (Intern), Van Nong, N. (Intern), Le, T. H. (Intern), Balke, B. (Ekstern), Han, L. (Intern), Jensen Hedegaard, E. M. (Ekstern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 8
Pages: 594-601
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Electronic Materials
Volume: 45
Issue number: 1
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.586 SNIP 0.844 CiteScore 1.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.69 SNIP 1.083 CiteScore 1.82
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.713 SNIP 1.109 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.866 SNIP 1.318 CiteScore 1.74
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.841 SNIP 1.157 CiteScore 1.66
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.777 SNIP 1.049
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.927 SNIP 1.148
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.875 SNIP 0.961
Scopus rating (2007): SJR 0.897 SNIP 1.067
Scopus rating (2006): SJR 1.041 SNIP 1.241
Scopus rating (2005): SJR 1.12 SNIP 1.236
Scopus rating (2004): SJR 1.093 SNIP 1.232
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.174 SNIP 1.161
On the chemical synthesis route to bulk-scale skutterudite materials

In this article an alternative high yield route for the synthesis of CoSb₃-based unfilled skutterudites is presented. Using low-melting temperature salts of the constituents, melting and mixing them homogeneously in a hydrophobic liquid with postprocessing of the powders we achieve a more intimately mixed alloy compared to the conventional melting and metallurgical processes. The proposed method consists of a fast and low-temperature processing step followed by a thermochemical post-processing step, compared to the conventional methods of fabricating skutterudites, which require high temperatures and long processing times. Several structural characterization techniques were used to assess the mechanism of synthesis, verify the purity of the material as well as the reproducibility of the process. Detailed analysis and results are presented in support of the proposed process. Additionally, compaction of the powders with SPS technique provided a safe route to maintaining the nanopowder size and achieving low thermal conductivity (3 W/mK). The proposed method can easily be scaled up and adopted by the industry.
Operational stability of large scale OPV modules: interfaces, materials selection and stack design

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Roth, B. (Intern), Krebs, F. C. (Intern), Søndergaard, R. R. (Intern)
Number of pages: 135
Publication date: 2016

Publication information
Place of publication: Roskilde, Denmark
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Electronic): 978-87-92986-49-8
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD_thesis_Berenger_Roth_print_red.pdf

Relations
Projects:
Operational stability of large scale OPV modules: interfaces, materials selection and stack design

Optimally segmented magnetic structures
We present a semi-analytical algorithm for magnet design problems, which calculates the optimal way to subdivide a given design region into uniformly magnetized segments. The availability of powerful rare-earth magnetic materials such as Nd-Fe-B has broadened the range of applications of permanent magnets[1][2]. However, the powerful rare-earth magnets are generally expensive, so both the scientific and industrial communities have devoted a lot of effort into developing suitable
design methods. Even so, many magnet optimization algorithms either are based on heuristic approaches[3], or are applicable only to analytically solvable geometries[4]. In addition, some questions remained fundamentally unanswered, such as how to segment a given design into N uniformly magnetized pieces. Our method calculates the globally optimal shape and magnetization direction of each segment inside a certain design area with an optional constraint on the total amount of magnetic material. The method can be applied to any objective functional which is linear respect to the field, and with any combination of linear materials. Being based on an analytical-optimization approach, the algorithm is not computationally intensive and provides the global optimum with respect to the considered problem without the need for a starting guess. The approach can be used in combination with finite element method calculations, and can therefore be applied also to problems for which an analytical solution to the magnetic field is not available. We will illustrate the results for magnet design problems from different areas, such as electric motors/generators (as the example in the picture), beam focusing for particle accelerators and magnetic refrigeration devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Number of pages: 3
Publication date: 2016
Event: Abstract from 13th Joint MMM-Intermag Conference, San Diego, CA, United States.
Main Research Area: Technical/natural sciences
Segmentation, Optimization, Analytical, FEM
Electronic versions:
Optimally_segmented_magnetic_structures.pdf
Source: PublicationPreSubmission
Source-ID: 118674328
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Optimally segmented permanent magnet structures
We present an optimization approach which can be employed to calculate the globally optimal segmentation of a two-dimensional magnetic system into uniformly magnetized pieces. For each segment the algorithm calculates the optimal shape and the optimal direction of the remanent flux density vector, with respect to a linear objective functional. We illustrate the approach with results for magnet design problems from different areas, such as a permanent magnet electric motor, a beam focusing quadrupole magnet for particle accelerators and a rotary device for magnetic refrigeration.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences
Publication information
Journal: IEEE Transactions on Magnetics
Volume: 52
Issue number: 12
Article number: 7210306
ISSN (Print): 0018-9464
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.48 SNIP 0.915 CiteScore 1.47
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.565 SNIP 1.207 CiteScore 1.77
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.715 SNIP 1.491 CiteScore 1.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Optimising Magnetostatic Assemblies

The aim of this thesis is to investigate a framework to design and optimise magnetostatic systems. Over the course of the last decades the range of applications of permanent magnets expanded considerably, thanks to the development of powerful rare-earth permanent magnets. Concurrently, the research on methods to optimise permanent magnet based magnetic systems intensified. The increase in computational power, and the emergence of new optimisation algorithms provided new instruments for the design of magnetic systems. All these factor contribute in making the optimisation of magnetic systems a very lively sector of modern research.

The main focus of this work are magnetic systems based on permanent magnets, although hybrid systems combining permanent magnets with electromagnets are also considered. Many optimisation approaches presented here are derived within a framework based on the reciprocity theorem. This theorem formulates an energy equivalence principle with several implications concerning the optimisation of objective functionals that are linear with respect to the magnetic field. Linear functionals represent different optimisation goals, e.g. maximising a certain component of the field averaged over a region of space. In general, a linear functional can be expressed as the integral over a given region of the scalar product between the magnetic field and an arbitrarily defined objective vector field. It has been known for some time that the
The reciprocity theorem can be used to determine the optimal remanence distribution with respect to a linear objective functional. Additionally, it is shown here that the same formalism can be applied to the optimisation of the geometry of magnetic systems. Specifically, the border separating the permanent magnet from regions occupied by air or soft magnetic material can be optimised within this framework. Since in the practice most structures are realized by assembling uniformly magnetized pieces of permanent magnet, it is relevant to address the question of how a given region of space is best subdivided. This problem is investigated here within the framework of the reciprocity theorem. Analytical derivations will be used to show that, for segmentations controlled by a single parameter, the globally optimal solution to this problem can be determined for almost arbitrary geometries. The case of segmentations depending by two parameters has been approached employing a heuristic algorithm, which led to new design concepts. Some of the procedures developed for linear objective functionals have been extended to non-linear objectives, by employing iterative techniques. Even though most the optimality results discussed in this work have been derived analytically, the different approaches have been implemented in combination with finite element methods, resulting in flexible and computationally efficient algorithms. Most of the optimisation approaches could only be proven under the assumption of linear magnetic behavior. The last part of this thesis also investigates some of the effects on the performance of magnetic systems, due to non-linear magnetic phenomena. In particular, the non-linear demagnetization effects caused by the finite coercivity of the permanent magnet material will be examined.

All the optimisation techniques will be illustrated with example magnetic systems for different applications, thus showing the versatility and efficacy of the various approaches. The Halbach cylinder geometry, relevant for many applications, will be often used as example, also because of the many symmetries and optimality properties exhibited by this geometry. Despite the fact that this system has already been subject of many publications, some of the aspects considered in this thesis have not been investigated before. The ultimate goal of the PhD project is to apply the optimisation techniques developed during this research to the design of the magnetic system for the prototype of heat pump based on the magnetocaloric effect. Magnetic systems for room temperature magnetic refrigeration will thus frequently be used as illustrative examples along the course of this thesis.

Primarily because of the theoretical relevance of linear functionals, the results presented here lead to a deeper understanding of the magnet optimisation process. One of the perspectives considered in this work is the trade-off between field intensity and field quality, as the choice of a particular optimisation approach may favour one or the other. The general framework discussed here provides a set of useful tools aiding the magnet design process. This research also opened new scientific questions which would be worth investigating in future studies.
Optimization of Multi-layer Active Magnetic Regenerator towards Compact and Efficient Refrigeration

Magnetic refrigerators can theoretically be more efficient than current vapor compression systems and use no vapor refrigerants with global warming potential. The core component, the active magnetic regenerator (AMR) operates based on the magnetocaloric effect of magnetic materials and the heat regeneration processes of periodic fluid blows. Magnetocaloric materials with a first order phase transition (FOPT) are suitable to realize a higher cooling capacity than commonly used gadolinium, but layering such materials is necessary, due to a large isothermal entropy change ($\Delta S_m$) in a narrow region around their Curie temperature. Simulations are implemented to investigate how to layer the FOPT materials for obtaining higher cooling capacity. Moreover, based on entropy generation minimization, optimization of the regenerator geometry and related operating parameters is presented for improving the AMR efficiency. In addition, simulations are carried out to investigate the potential of applying nanofluid in future magnetic refrigerators.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems (ECOS 2016)
Article number: PAP-433
Main Research Area: Technical/natural sciences
Conference: 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, Portorož, Slovenia, 19/06/2016 - 19/06/2016
Electronic versions:
Optimization_of_Multi_layer_Active.pdf

Bibliographical note
Presentation section: Refrigeration & air conditioning; Heat pumps

Optimization of the Public Buildings Energy Supply: the case of the school in Koprivnica

There is a rising interest in the improvement of energy efficiency in public buildings nowadays at the EU level. Increasing energy efficiency can lead to both better thermal comfort, as well as net savings on energy bills. Furthermore, the right choice of energy source can lead to large savings in CO2 emissions. Recently, there have been a lot of projects in Croatia concerning the renovation of schools. However, many of them do not take the holistic approach during the refurbishment projects. They rather focus on a partial solution, focusing only on heating or heating and power supply. Furthermore, the choice of heating furnaces is often based on old and inaccurate data, without any mid or long term planning. In order to solve this issue, a simple to use continuous linear optimization model has been developed, which calculates the best investment options for heating, cooling and power supply. The model has a variety of choices and chooses the optimal one based on the external conditions entered, such as hourly temperatures, wind speed and global insolation. The model uses hourly time steps during one year, while the objective function of the developed model is to minimize net present value of the project. The model was validated on a case of Antun Nemcic Gostovinski primary school in Koprivnica, Croatia. The school has 728 pupils and 77 employees and is open from 08 AM to 08 PM every working day. It also has two adjacent gyms, kitchen and the library. The model showed that significant savings could be achieved by taking a holistic approach during the refurbishment of the building, at the same time increasing thermal comfort of the students and employees. Finally, the developed model would be easy to adapt to any other similar public building, which could lead to further savings in energy consumption.

General information
State: Published
Outdoor fate and environmental impact of polymer solar cells through leaching and emission to rainwater and soil

The emission of silver and zinc to the aqueous environment (rain, fog, dew) from polymer solar cells installed outdoors is presented. Studies included pristine solar cells and solar cells subjected to mechanical damage under natural weather conditions in Denmark. We find the emission of silver and zinc to the environment through precipitated water for damaged solar cells, and also observed failure and emission from an initially undamaged device in an experiment that endured for 6 months. In the case of the damaged cells, we found that the drinking water limits for Ag were only exceeded on a few single days. We also progressed our studies to include end-of-life management. To assess the implications of improper practices (uncontrolled disposal, landfilling) at the end-of-life, we buried different OPV types in intact and damaged forms in soil columns. In the case of high Ag emission (shredded cells), the potential for migration was confirmed, even though the soil was found to exhibit sequestration of silver. We conclude that recycling of Ag at the end-of-life is mandatory from an environmental point of view.
Oxygen permeation flux through 10Sc1YSZ-MnCo2O4 asymmetric membranes prepared by two-step sintering

Asymmetric membranes based on a dual phase composite consisting of (Y2O3)0.01(Sc2O3)0.10(ZrO2)0.89 (10Sc1YSZ) as ionic conductor and MnCo2O4 as electronic conductor were prepared and characterized with respect to sinterability, microstructure and oxygen transport properties. The composite membranes were prepared by tape casting, lamination and fired in a two-step sintering process. Microstructural analysis showed that a gastight thin membrane layer with the desired ratio of ionic/electronic conducting phases could be fabricated. Oxygen permeation fluxes across the 10Sc1YSZ/MnCo2O4 (70/30 vol%) composite membrane were measured from 750 to 940 degrees C using air or pure oxygen as feed gases and N2 or CO2 as sweep gases. Fluxes up to 2.3 mlN min⁻¹ cm⁻² were obtained for the 7 μm thick membrane. A degradation test over 1730 h showed an initial degradation of 21% during the first 1100 h after which stable performance was achieved. The observed degradation is attributed to coarsening of the infiltrated catalyst. (C) 2016 Elsevier B.V. All rights reserved.
We study the oxygen reduction reaction (ORR), the catalytic process occurring at the cathode in fuel cells, on Pt layers prepared by electrodeposition onto an Au substrate. Using a nominal Pt layer by layer deposition method previously proposed, imperfect layers of Pt on Au are obtained. The ORR on deposited Pt layers decreases with increasing Pt thickness. In the submonolayer region, however, the ORR activity is superior to that of bulk Pt. Using density functional theory (DFT) calculations, we correlate the observed activity trend to strain, ligand, and ensemble effects. At submonolayer coverage certain atom configurations weaken the binding energies of reaction intermediates due to a ligand and ensemble effect, thus effectively increasing the ORR activity. At higher Pt coverage the activity is governed by a strain effect, which lowers the activity by decreasing the oxidation potential of water. This study is a nice example of how the influence of strain, ligand, and ensemble effects on the ORR can be deconvoluted.
Patterning and Conductivity Modulation of Conductive Polymers by UV Light Exposure
A novel patterning technique of conductive polymers produced by vapor phase polymerization is demonstrated. The method involves exposing an oxidant film to UV light which changes the local chemical environment of the oxidant and subsequently the polymerization kinetics. This procedure is used to control the conductivity in the conjugated polymer poly(3,4-ethylenedioxythiophene):tosylate by more than six orders of magnitude in addition to producing high-resolution patterns and optical gradients. The mechanism behind the modulation in the polymerization kinetics by UV light irradiation as well as the properties of the resulting polymer are investigated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linkoping University, University of South Australia
Number of pages: 11
Pages: 6950-6960
Publication date: 2016
Main Research Area: Technical/natural sciences
Lithium-ion batteries (LIBs) find widespread use for electricity storage, from portable devices such as smart phones to electric vehicles (EV), because of their high energy density and design flexibility. However, limited lifetime is still a challenge for several LIB materials. Specifically, the detailed coupling between degradation mechanisms and battery usage is not fully understood, which impede lifetime improvements. To understand the degradation mechanisms and increase the performance of these materials, the development of improved characterization methods is crucial. This PhD thesis focuses on the thorough analysis of degradation mechanism in LIBs, trying to relate morphological and structural changes in Lithium-ion battery electrodes to performance degradation observed during electrode cycling. Degradation mechanisms in laboratory scale LFP cathodes were correlated with the degradation mechanisms observed in commercial LIBs. The structural and morphological changes in cycled laboratory LFP cathodes were studied by low-kV FIB/SEM Tomography and TEM analysis and related to the electrode performance using Electrochemical Impedance Spectroscopy (EIS). The two main degradation processes observed by microscopy analysis in the aged electrode were cracking of LFP particles and agglomeration of carbon black (CB) additive. The increased heterogeneity of the CB network reduces the electron percolation throughout the porous electrode, thereby decreasing the amount of electrochemically active LFP particles. The electron resistivity was quantified with the EIS analysis using a Transmission Line Model (TLM) developed for porous LFP electrodes. Similar TLM models were applied for the analysis of the polarization processes in a commercial LFP and graphite electrodes. The microscopy analysis of the electrodes showed the presence of
carbonaceous agglomerates on the electrode/electrolyte interfaces. The agglomerates are expected to increase the ionic resistance and be related to loss of lithium inventory (LLI).

**Performance Factors and Sulfur Tolerance of Metal Supported Solid Oxide Fuel Cells with Nanostructured Ni:GDC Infiltrated Anodes**

Two metal supported solid oxide fuel cells (active area 16 cm²) with nanostructured Ni:GDC infiltrated anodes, possessing different anode and support microstructures were studied in respect to sulfur tolerance at an operating temperature of 650°C. The studied MS-SOFCs are based on ferretic stainless steel (FeCr) and showed excellent performance characteristics at 650°C with fuel utilization corrected area specific resistances of 0.35 Ωcm² and 0.7 Ωcm² respectively. The sulfur tolerance testing was performed by periodic addition of 2, 5, and 10 ppm H₂S in hydrogen based fuel under galvanostatic operation at a current load of 0.25 Acm⁻². The results were compared with literature on the sulfur tolerance of conventional SOFC Ni/YSZ cermet anode. The comparison in terms of absolute cell resistance increase and relative anode polarization resistance increase indicates, that the nanostructured Ni:GDC MS-SOFC based anode is significantly more sulfur tolerant than the conventional Ni/YSZ cermet anode. Furthermore, it was shown that the believed extension of the electrochemical three-phase-boundary reaction zone in the presence of GDC must be very limited and cannot account for the higher sulfur tolerance of GDC modified SOFC anodes.
Performance of Halbach magnet arrays with finite coercivity

A numerical method to study the effect of finite coercivity on the Halbach cylinder geometry is presented. Despite the fact that the analytical solution available for this geometry does not set any limit to the maximum air gap flux density achievable, in real life the non-linear response of the magnetic material and the fact that the coercivity is not infinite will limit the attainable field. The presented method is able to predict when and where demagnetization will occur, and these predictions are compared with the analytical solution for the case of infinite coercivity. However, the approach presented here also allows quantification of the decrease in flux density and homogeneity for a partially demagnetized magnet. Moreover, the problem of how to realize a Halbach cylinder geometry using a mix of materials with different coercivities without altering the overall performance is addressed. Being based on a numerical approach, the presented method can be employed to analyze the demagnetization effects due to coercivity for any geometry, even when the analytical solution is not available.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Number of pages: 8
Pages: 369-376
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 407
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285 CiteScore 1.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Due to the attractive properties of nanoparticles because of their effective surface area, they have been studied widely. Nano-yttria-stabilized zirconia (n-YSZ) is a ceramic which has been scrutinized extensively in past years. Because of the different stability behavior of n-YSZ in comparison with bulk YSZ, a new phase diagram is needed for the n-YSZ system in order to identify stable phases under various conditions. In this study, a phase diagram for the n-YSZ system was provided to determine phase stability ranges at room temperature with respect to particle size and composition. The calculation of phase diagrams (CALPHAD) approach was applied to calculate the Gibbs energy of bulk YSZ. It was combined with the surface energy of each phase in the n-YSZ system, i.e. monoclinic, tetragonal, cubic, and amorphous, to produce the total Gibbs energy of each individual phase of the n-YSZ system. By applying the CALPHAD approach, a 3-D phase diagram for the n-YSZ system was established in which the stability range of each individual phase can be predicted based on the particle size, composition, and temperature.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Florida International University
Authors: Asadikiya, M. (Ekstern), Sabarou, H. (Ekstern), Chen, M. (Intern), Zhong, Y. (Ekstern)
Number of pages: 8
Pages: 17438-17445
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: R S C Advances
Volume: 6
Issue number: 21
ISSN (Print): 2046-2069
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Plasma diagnostics during magnetron sputtering of aluminum doped zinc oxide

Plasma parameters during magnetron sputtering of aluminum-doped zinc oxide are investigated with optical emission spectroscopy, electrostatic probes and mass spectrometry with the aim of understanding the role of negative ions of oxygen during the film growth and improving the uniformity of the film resistivity over the deposition area.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Micro- and Nanotechnology, Silicon Microtechnology, Electrofunctional materials
Authors: Stamate, E. (Intern), Crovetto, A. (Intern), Sanna, S. (Intern)
Pages: 327-328
Publication date: 2016

Host publication information
Title of host publication: Proceedings of 23rd Europhysics Conference on Atomic and Molecular Physics of Ionized Gases (ESCAMPIG XXIII)
Publisher: European Physical Society
Main Research Area: Technical/natural sciences
Conference: 23rd Europhysics Conference on Atomic and Molecular Physics of Ionized Gases, Bratislava, Slovakia, 12/07/2016 - 12/07/2016

Platinum Iron Intermetallic Nanoparticles Supported on Carbon Formed In Situ by High-Pressure Pyrolysis for Efficient Oxygen Reduction

Carbon-supported PtFe alloy catalysts are synthesized by the one-step, high-temperature pyrolysis of Pt, Fe, and C precursors. As a result of the high temperature, the formed PtFe nanoparticles possess highly ordered, face-centered tetragonal, intermetallic structures with a mean size of \( \approx 11.8 \) nm. At 0.9 V versus the reversible hydrogen electrode, the PtFe nanoparticles show a 6.8 times higher specific activity than the reference Pt/C catalyst towards the oxygen reduction reaction (ORR) as well as excellent stability, most likely because of the durable intermetallic structure and the preleaching treatment of the catalyst. During these preliminary syntheses, we found that a portion of the PtFe nanoparticles is buried in the in situ formed carbon phase, which limits Pt utilization in the catalyst and results in a mass-specific activity equivalent to the commercial Pt/C catalyst. Moreover, the possible presence of other active sites, for example, FeN_\( x \) \_ CN_\( x \) \_ and carbon-encapsulated metal nanoparticles, and their contribution to the ORR performance of the catalyst are also investigated.
Playing with Light in Organic Thin-Film Solar Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Playing_with_Light.pdf
**Play with light in thin film organic materials: from nanoscale to smart windows**

**General information**
State: Published  
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials  
Authors: Pastorelli, F. (Intern)  
Publication date: 2016

**Publication information**
Media of output: Video  
Original language: English  
Publisher: DTU Energy  
Main Research Area: Technical/natural sciences  
Links: https://youtu.be/tb_Dq-OMPnQ

**Bibliographical note**
Invited talk  
Source: PublicationPreSubmission  
Source-ID: 127807154

**Polaronic motion of self-trapped holes in silver halides**

**General information**
State: Published  
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad de Cantabria  
Authors: García Lastra, J. M. (Intern), García-Fernandez, P. (Ekstern), Loftager, S. (Intern), Aramburu, J. (Ekstern), Moreno, M. (Ekstern)  
Number of pages: 1  
Publication date: 2016  
Event: Abstract from International Conference on Defects in Insulating Materials (ICDIM 2016), Lyon, France.  
Main Research Area: Technical/natural sciences  
Electronic versions: Polaronic_motion.pdf  
Source: PublicationPreSubmission  
Source-ID: 128083480

**Polybenzimidazole Membranes by Post Acid Doping**

**General information**
State: Published  
Organisations: Department of Energy Conversion and Storage, Proton conductors  
Authors: Aili, D. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)  
Pages: 195-215  
Publication date: 2016  
Host publication information  
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives  
Place of publication: Switzerland  
Publisher: Springer  
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.  
ISBN (Print): 978-3-319-17081-7  
ISBN (Electronic): 978-3-319-17082-4  
Chapter: 9
Polybenzimidazole membranes for zero gap alkaline electrolysis cells
Membranes of m-PBI doped in KOH (aq), 15-35 wt%, show high ionic conductivity in the temperature range 20-80 °C. In electrolysis cells with nickel foam electrodes m-PBI membranes provide low internal resistance. With a 60 µm membrane at 80°C in 20 wt% KOH, 1000 mA/cm² is achieved at 2.25.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kraglund, M. R. (Intern), Aili, D. (Intern), Christensen, E. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at The 21st World Hydrogen Energy Conference (WHEC), Zaragoza, Spain.
Main Research Area: Technical/natural sciences
Electronic versions: WHEC2016_polbenzimidazole_membranes_for_zero_gap_alkaline_electrolysis_cells.pdf
Source: PublicationPreSubmission
Source-ID: 125388571
Publication: Research - peer-review › Poster – Annual report year: 2016

Polymer materials for roll coated solar cells: strategies to improve performance and stability
Solar cells are among the renewable energy technologies with a large potential in terms of solar energy availability. The solar cells based on conjugated polymers belong to the third generation of this technology and their attractive features include a fast and cheap solution-processed production. At DTU Energy the focus is the roll-to-roll coating process of these materials in order to reach large area devices, as the processability and scalability of the technology is an important factor. The process ability using roll-coating techniques and the stability of the used materials can be crucial. Therefore this project focuses on the synthesis of conjugated polymers and their application in roll-coated polymer solar cells. The first part of this project aims at using a screening strategy to find suitable polymer candidates for well performing solution processed polymer solar cells. A large number of polymers was screened by applying them in roll-coated solar cells and their performance, stability and number of synthetic steps was compared, to find promising candidates. In the end seven polymers with a sufficient efficiency were found to behave in a higher or in similar manner as poly(3-hexylthiophene). Further polymers were prepared based on well-performing benzothiadiazole and thiophene based polymers with different incorporation ratios of these monomers. The incorporation ratio has different effects on the polymer properties and the performance and stability of the corresponding roll-coated devices. The best efficiency was achieved with a polymer by using an incorporation of four thiophenes in the repeating unit. The second part of the work aims at using a known strategy to improve the solar cells stability. Three of the polymers from the polymer screening were therefore partly modified with stabilizing side chains, 2-phenetyl and 2-ethanol, respectively, to influence especially the device stability but also the performance. For most modifications a decrease of the solar cell efficiency was observed. The incorporation of 10% of these side chains show improvements of the stability of devices in a minor degree with a variation in the photo- and thermal stability. In addition to the use of different side chains, the impact of different positioning of one side chain was investigated, showing that the incorporation onto the acceptor or donor unit of the polymer showed a degradation or improvement of the resulting properties. In addition, the approach of side chain removable on polythiophene was compared in terms of optical properties and morphologies of two polymers with different (thermal or acidic) cleavage processes. It was found that their properties were not the same and therefore different results from the corresponding solar cells can be expected.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Heckler, I. M. (Intern), Bundgaard, E. (Intern)
Number of pages: 234
Publication date: 2016

Publication information
Place of publication: Kgs. Lyngby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-59-7
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Poly(vinylpyrrolidone) as dispersing agent for cerium-gadolinium oxide (CGO) suspensions

The behaviour of selected poly(vinylpyrrolidone) grades to act as dispersant for ethanol-based cerium gadolinium oxide suspensions was investigated and related to the molecular weight characteristics. The number, weight, and z-average molecular weights $M_n$, $M_w$, and $M_z$ were determined by gel permeation chromatography and then used in a numerical method to evaluate the viscosity average molecular weight ($M_v$) via an empirically modified Mark–Houwink–Sakurada (MHS) equation. The MHS equation parameters ($a$ and $K$) and the polydispersity correction factor ($q_{MHS}$) were also evaluated. Three grades with different molecular weight features were selected and further studied as dispersants by means of rheology. Despite the differences, only slight shifts in the amount of polymer required for achieving fully stabilized dispersions were observed, whereas comparable packing properties were obtained. This was explained as an effect of the polydispersity, expressed as $q_{MHS}$.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Self-Organized Nanoporous Materials, Mixed Conductors
Authors: Marani, D. (Intern), Sudireddy, B. R. (Intern), Nielsen, L. (Intern), Ndoni, S. (Intern), Kiebach, W. (Intern)
Pages: 1098-1106
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Science
Volume: 51
Issue number: 2
ISSN (Print): 0022-2461
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.762 SNIP 1.064
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.811 SNIP 1.081 CiteScore 2.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.985 SNIP 1.431 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.933 SNIP 1.472 CiteScore 2.36
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.991 SNIP 1.407 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.941 SNIP 1.393 CiteScore 2.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.965 SNIP 1.097
Portable and wireless IV-curve tracer for >5 kV organic photovoltaic modules

The practical design of a wirelessly controlled portable IV-curve tracer based on a capacitive load is described. The design is optimized for the measurement of solar cell modules presenting a high open circuit voltage of up to 6 kV and a low short circuit current below 100 mA. The portable IV-tracer allows for on-site/in-situ characterization of large modules under real operating conditions and enables fast detection of potential failure of anomalies in electrical behavior. Currently available electronic loads only handle voltages up to around 1 kV. To overcome cost and safety issues related to high voltage applications, the design is based on low cost components, battery-based isolated supply and wireless communication. A prototype has been implemented and field tested for characterization of different organic photovoltaic modules (OPV) made according to the infinity concept with a large number of serially connected single junctions (~7,450 single junctions) presenting open circuit voltages up to 5.6 kV.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technical University of Cartagena
Number of pages: 6
Pages: 60-65
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Solar Energy Materials and Solar Cells
Volume: 151
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.524 SNIP 2.121
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.991 SNIP 1.977
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.654 SNIP 1.458
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.359 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.447 SNIP 1.799
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.141 SNIP 1.619
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.932 SNIP 1.178
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.992 SNIP 1.34
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.042 SNIP 1.114
Scopus rating (2001): SJR 0.896 SNIP 1.235
Scopus rating (2000): SJR 0.828 SNIP 0.986
Scopus rating (1999): SJR 0.701 SNIP 0.75
Original language: English
Fast recording, High voltage, IV-tracer, Organic/polymer solar cells, Wireless control
DOIs:
10.1016/j.solmat.2016.02.012
Source: FindIt
Source-ID: 277406568
Publication: Research - peer-review › Journal article – Annual report year: 2016
Potato extract as reducing agent and stabiliser in a facile green one-step synthesis of ZnO nanoparticles

A facile green recipe was developed to synthesise highly pure, safe and durable zinc oxide nanoparticles (ZnO NPs) using homemade starch-rich potato extract. The ZnO NPs were synthesised using zinc nitrate and potato extract, and the whole reaction is carried out for 30 min at 80 °C. In the synthesis, starch-rich potato extract acted as the reducing agent and as a stabilising layer on freshly formed ZnO NPs. Hexagonal (wurtzite) shaped ZnO NPs with size about 20 ± 1.2 nm were synthesised and characterised using X-ray diffraction, transition electron microscope and scanning microscopy analyses. Fourier transform infrared spectral analysis indicated that highly pure ZnO nanopowders were obtained at higher temperatures. The use of environmentally benign and renewable material as the respective reducing and protecting agents, starch-rich potato extract, as well as a gentle solvent medium (H2O), offered a simple and quite efficient procedure for the synthesis of ZnO NPs in neutral medium with promising potential for biological and biomedical applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Khorramshahr University of Marine Science and Technology, University of Ohio, Ahvaz Jundishapur University of Medical Sciences
Authors: Buazar, F. (Ekstern), Bavi, M. (Ekstern), Kroushawi, F. (Intern), Halvani, M. (Ekstern), Khaledi-Nasab, A. (Ekstern), Hossieni, S. (Ekstern)
Pages: 175-184
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Experimental Nanoscience
Volume: 11
Issue number: 3
ISSN (Print): 1745-8080
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 0.91 SJR 0.244 SNIP 0.412
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.199 SNIP 0.362 CiteScore 0.71
Scopus rating (2014): SJR 0.279 SNIP 0.443 CiteScore 0.74
Scopus rating (2013): SJR 0.334 SNIP 0.53 CiteScore 0.85
Scopus rating (2012): SJR 0.348 SNIP 0.509 CiteScore 0.89
Scopus rating (2011): SJR 0.39 SNIP 0.633 CiteScore 1.16
Scopus rating (2010): SJR 0.312 SNIP 0.406
Scopus rating (2009): SJR 0.183 SNIP 0.212
Scopus rating (2008): SJR 0.216 SNIP 0.267
Original language: English
Crystal structure, green synthesis, nanostructures, potato extract, ZnO, Biological materials, Crystal structure, Medical applications, Nanoparticles, Nanostructures, Spectrum analysis, Starch, X ray diffraction, Zinc, Zinc oxide, Zinc sulfide, Biomedical applications, Environmentally benign, Fourier transform infra reds, Green synthesis, Scanning microscopy, Zinc oxide nanoparticles, Synthesis (chemical)
Electronic versions:
Potato_extract_as_reducing_agent.pdf
DOIs:
10.1080/17458080.2015.1039610
Source: FindIt
Source-ID: 274980107
Publication: Research - peer-review › Journal article – Annual report year: 2016

Preparation and Characterization of Cathode Materials for Lithium-Oxygen Batteries

A possible future battery type is the Li-air battery which theoretically has the potential of reaching gravimetric energy densities close to those of gasoline. The Li-air battery is discharged by the reaction of Li-ions and oxygen, drawn from the air, reacting at the battery cathode to form Li2O2. The type of cathode material affects the battery discharge capacity and charging potential and with a carbon based cathode many questions are still unanswered. The focus of this Ph.D. project has been the synthesis of reduced graphene oxide as well as the investigation of the effect of reduced graphene oxide as a cathode material, combined with in situ investigations of the formation of decomposition products in and on the cathode. The reduced graphene oxide was synthesized by the modified Hummers method followed by thermal reduction of graphene oxide, while both were investigated by in situ X-ray diffraction. This study revealed an early formation of graphene oxide, new graphene oxide diffraction peaks and an unidentified crystal phase along with a disordered stage of thethermal reduction of graphene oxide. The oxidation time effect on graphene oxide, synthesized by the modified
Hummers method, and the following chemically and thermal reduced graphene oxide was investigated. This revealed that trends introduced by changes in oxidation time were observed not only for the graphene oxide but also transcended to both types of reduced graphene oxide. Furthermore the change in oxidation time affected the discharge capacity of the battery as well as the charging potential. In situ X-ray diffraction studies on carbon black cathodes in a capillary battery showed the formation of crystalline Li$_2$O$_2$ on the first discharge cycle, the intensity of Li$_2$O$_2$ on the second discharge cycle was however diminished. The study furthermore showed how X-rays may affect the Li-O$_2$ battery, displaying how in situ studies may be invasive. An in situ X-ray diffraction study of a reduced graphene oxide cathode showed formation of both LiOH and Li$_2$O$_2$, which also was observed in cells with and without addition of water by XPS. The addition of water to the electrolyte gave indications of additional reactions taking place in the cell. The information provided in this study is useful for a better understanding of reduced graphene oxide both in regards to synthesis and as cathode material in Li-air batteries. The thesis illuminates the importance of considering the synthesis of reduced graphene oxide as this seems to be couple to the abilities as cathode materials in Li-air batteries. It furthermore introduces two types of capillary battery designs optimized for Li-air and in situ X-ray diffraction, but with possibilities within metal-air batteries in general, and it opens up for a discussion of how invasive in situ methods may be.
Preparation and characterization of Sc doped MgB$_2$ wires

The *in-situ* technique was used to manufacture scandium (Sc) doped MgB$_2$ wires in a composite Cu–Nb sheath. After reaction at 700 °C, at most 1 at.% Mg was replaced by Sc in the MgB$_2$ phase, without significant influence on its...
superconducting transition temperature. For higher Sc concentrations in the nominal composition, the formation of Sc-rich impurity phases was evidenced by SEM/EDS observations. The critical current density and accommodation field of the wires are weakly dependent on the Sc content. It is believed that these effects are related more to modifications of the thermal behaviour of the precursor powders revealed by DTA measurements than to actual doping. The best performance was obtained in a wire with Mg:Sc = 0.995±0.005 atomic ratio.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Polytechnical University of Bucharest
Authors: Grivel, J. (Intern), Burdusel, M. (Ekstern)
Number of pages: 8
Pages: 65-72
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica C: Superconductivity and its Applications
Volume: 528
ISSN (Print): 0921-4534
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.575 SNIP 0.924 CiteScore 1.14
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.446 SNIP 0.888 CiteScore 0.99
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.497 SNIP 0.83 CiteScore 0.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.439 SNIP 0.7 CiteScore 0.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.55 SNIP 0.621 CiteScore 0.79
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.652 SNIP 0.607 CiteScore 0.94
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.63 SNIP 0.631
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.412 SNIP 0.56
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.67 SNIP 0.576
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.532 SNIP 0.716
Scopus rating (2006): SJR 0.667 SNIP 0.556
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.793 SNIP 0.656
Web of Science (2005): Indexed yes
Preparation, structure study and electrochemistry of layered $\text{H}_2\text{V}_3\text{O}_8$ materials: High capacity lithium-ion battery cathode

The present study explores $\text{H}_2\text{V}_3\text{O}_8$ as high capacity cathode material for lithium-ion batteries (LIB’s). Despite having high discharge capacity, $\text{H}_2\text{V}_3\text{O}_8$ material suffers from poor electrochemical stability for prolonged cycle life. Ultra-long $\text{H}_2\text{V}_3\text{O}_8$ nanobelts with ordered crystallographic patterns are synthesized via a hydrothermal process to mitigate this problem. The growth of the crystal is facile along [001] direction, and the most common surface is (001) as suggested by Wulff construction study. Electrochemical performance of $\text{H}_2\text{V}_3\text{O}_8$ cathode is tested against Li/Li+ at various current rates. At 50 mA g$^{-1}$ current rate, it delivers a discharge capacity of 308 mAh g$^{-1}$, whereas, at 3000 mA g$^{-1}$, an initial discharge capacity of 144 mAh g$^{-1}$ is observed and stabilized at 100 mAh g$^{-1}$ till 500 cycles. Further, the density functional theory (DFT) based simulations study of both the pristine and lithiated phase of $\text{H}_2\text{V}_3\text{O}_8$ cathode materials is undertaken. DFT study reveals the presence of hydrogen as hydroxyl unit in the framework of the host. In correlation, the magnetic property of vanadium atoms is examined in detail with through partial density of states (PDOS) calculation during three stage lithiation processes and evaluating various potential steps involved in lithium insertion.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Center for Study of Science, Technology and Policy, Indian Institute of Technology, Bombay
Authors: Sarkar, S. (Ekstern), Bhowmik, A. (Intern), Pan, J. (Intern), Bharadwaj, M. D. (Ekstern), Mitra, S. (Ekstern)
Number of pages: 11
Pages: 179-189
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Power Sources
Volume: 329
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
Pressurized Operation of a Planar Solid Oxide Cell Stack

Solid oxide cells (SOCs) can be operated either as fuel cells (SOFC) to convert fuels to electricity or as electrolyzers (SOEC) to convert electricity to fuels such as hydrogen or methane. Pressurized operation of SOCs provide several benefits on both cell and system level. If successfully matured, pressurized SOEC based electrolyzers can become more efficient both energy- and cost-wise than PEM and Alkaline systems. Pressurization of SOFCs can significantly increase the cell power density and reduce the size of auxiliary components. In the present study, a SOC stack was successfully operated at pressures up to 25 bar. The pressure dependency of the measured current-voltage (I-V) curves and impedance spectra on the SOC stack are analyzed and the relation between various system parameters and pressure is derived. With increasing pressure the open circuit voltage (OCV) and the reaction kinetics (electrode performance) increases for thermodynamic and kinetic reasons, respectively. Further, the summit frequency of the gas concentration impedance arc and the pressure difference across the stack and heat exchangers is seen to decrease with increasing pressure following a power-law expression. Finally a durability test was conducted at 10 bar.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Jensen, S. H. (Intern), Sun, X. (Intern), Ebbesen, S. D. (Intern), Chen, M. (Intern)
Number of pages: 14
Pages: 205–218
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 16
Issue number: 2
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.699 SNIP 0.787 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.629 SNIP 0.816 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.841 SNIP 0.848 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.25 SNIP 1.008 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.656 SNIP 1.238 CiteScore 3.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.632 SNIP 1.243
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.368 SNIP 1.12
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.523 SNIP 1.226
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.349 SNIP 1.086
Scopus rating (2006): SJR 1.194 SNIP 1.228
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.45 SNIP 0.501
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.232 SNIP 0.215
Web of Science (2004): Indexed yes
Web of Science (2001): Indexed yes
Original language: English
Durability, Electrochemical Impedance Spectroscopy, I-V curves, Planar, Pressure, Solid Oxide Cell, Stack, Electrochemical impedance spectroscopy
Printable luminescent down shifter for enhancing efficiency and stability of organic photovoltaics

The proof of concept of using luminescent down shifting (LDS) layers as alternative UV filters for P3HT:PCBM OPVs is demonstrated using a lanthanide-based metal complex. The results are verified using a combination of indoor light soaking, with single cell devices, and outdoor performance monitoring, using a 16-cell monolithically connected OPV module. By applying the LDS layer, a ~5% relative enhancement in photocurrent is observed for both sets of devices. More significantly, indoor light soaking tests on single cell devices without encapsulation showed an 850% enhancement in the measured half-life (T50%). The OPV modules were encapsulated and tested for outdoor stability over a 70 day period in the Negev desert, Israel. The modules made with the LDS filter are shown to match the stability of those made with a commercial UV filter and outperform the modules with no filter applied, with a 51% enhancement in the measured stability (T75%). Significantly, the work provides clear experimental evidence that the LDS layer can act as a UV filter in OPVs without compromising the efficiency of the solar cell, thus providing an added benefit over commercial UV filters.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Bangor University, Ben-Gurion University of the Negev, Swansea University
Authors: Kettle, J. (Ekstern), Bristow, N. (Ekstern), Gethin, D. (Ekstern), Tehrani, Z. (Ekstern), Moudam, O. (Ekstern), Li, B. (Ekstern), Katz, E. (Ekstern), Benatto, G. A. D. R. (Intern), Krebs, F. C. (Intern)
Pages: 481–487
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 144
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.524 SNIP 2.121
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.991 SNIP 1.977
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.654 SNIP 1.458
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.359 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.447 SNIP 1.799
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.141 SNIP 1.619
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.932 SNIP 1.178
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.992 SNIP 1.34
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.042 SNIP 1.114
Scopus rating (2001): SJR 0.896 SNIP 1.235
Scopus rating (2000): SJR 0.828 SNIP 0.986
Scopus rating (1999): SJR 0.701 SNIP 0.75
Original language: English
Organic photovoltaics, Degradation, Outdoor performance, UV filter, Luminescent material
DOIs:
10.1016/j.solmat.2015.09.037
Source: PublicationPreSubmission
Source-ID: 117917685
Publication: Research - peer-review › Journal article – Annual report year: 2016

Probing the active site structures of iron-based ORR catalysts

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Hu, Y. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2771
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/38/2771.abstract?sid=9220813d-2d81-4fd3-834c-3acb5da2f24f
Source: PublicationPreSubmission
Source-ID: 127806385
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Promising bulk nanostructured Cu₂Se thermoelectrics via high throughput and rapid chemical synthesis
A facile and high yield synthesis route was developed for the fabrication of bulk nanostructured copper selenide (Cu₂Se) with high thermoelectric efficiency. Starting from readily available precursor materials and by means of rapid and energy-efficient microwave-assisted thermolysis, nanopowders of Cu₂Se were synthesized. Powder samples and compacted pellets have been characterized in detail for their structural, microstructural and transport properties. α to β phase transition of Cu₂Se was confirmed using temperature dependent X-ray powder diffraction and differential scanning calorimetry analyses. Scanning electron microscopy analysis reveals the presence of secondary globular nanostructures
in the order of 200 nm consisting of <50 nm primary particles. High resolution transmission electron microscopy analysis confirmed the highly crystalline nature of the primary particles with irregular truncated morphology. Through a detailed investigation of different parameters in the compaction process, such as applied load, heating rate, and cooling profiles, pellets with preserved nanostructured grains were obtained. An applied load during the controlled cooling profile was demonstrated to have a big impact on the final thermoelectric efficiency of the consolidated pellets. A very high thermoelectric figure of merit (ZT) above 2 was obtained at 900 K for SPS-compacted Cu2Se nanopowders in the absence of the applied load during the controlled cooling step. The obtained ZT exceeds the state of the art in the temperature ranges above phase transition, approaching up to 25% improvement at 900 K. The results demonstrate the prominent improvement in ZT attributed both to the low thermal conductivity, as low as 0.38 W m−1 K−1 at 900 K, and the enhancement in the power factor of nanostructured Cu2Se. The proposed synthesis scheme as well as the consolidation could lead to reliable production of large scale thermoelectric nanopowders for niche applications.

Properties and Structure of the LiCl-films on Lithium Anodes in Liquid Cathodes

Lithium anodes passivated by LiCl layers in different types of liquid cathodes (catholytes) based on LiAlCl4 in SOCl2 or SO2 have been studied by means of impedance spectroscopy. The impedance spectra have been fitted with two equivalent circuits using a nonlinear least squares fit program. Information about the ionic conductivity and the structure of the layers has been extracted. A new physical model which is able to explain the circuit parameters is proposed. It
assumes that the LiCl-layer contains a large number of narrow tunnels and cracks filled with liquid catholyte. It is explained
why such tunnels probably are formed, and for a typical case it is shown that tunnels associated with most of the LiCl grain
boundaries of the fine crystalline layer near the Li surface are required in order to explain the impedance response. The
LiCl production rate and through this, the growth rate of the LiCl-layer, is limited by the electron conduc-tivity of the layer.
Micro-calorimetry data parallel with impedance spectra are used for determination of the electron conduc-tivity of the LiCl-
layer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Technical University of
Denmark
Authors: Mogensen, M. B. (Intern), Hennesø, E. (Ekstern)
Number of pages: 19
Pages: 519-534
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Chimica Slovenica
Volume: 63
Issue number: 3
ISSN (Print): 1318-0207
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.265 SNIP 0.501 CiteScore 0.93
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.29 SNIP 0.544 CiteScore 0.99
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.221 SNIP 0.534 CiteScore 0.75
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.279 SNIP 0.557 CiteScore 0.92
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.32 SNIP 0.512 CiteScore 1.07
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.373 SNIP 0.644 CiteScore 1.32
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.306 SNIP 0.57
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.305 SNIP 0.533
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.346 SNIP 0.615
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.379 SNIP 0.79
Scopus rating (2006): SJR 0.26 SNIP 0.587
Scopus rating (2005): SJR 0.215 SNIP 0.353
Scopus rating (2004): SJR 0.247 SNIP 0.375
Scopus rating (2003): SJR 0.288 SNIP 0.47
Scopus rating (2002): SJR 0.33 SNIP 0.579
Scopus rating (2001): SJR 0.324 SNIP 0.498
Scopus rating (2000): SJR 0.29 SNIP 0.361
Protic Organic Ionic Plastic Crystals: Fast Solid-State Proton Conductors

High temperature polymer electrolyte membrane fuel cells (PEMFCs) operating between 100 °C and 200 °C are desirable because they offer significant benefits, such as improved electrode kinetics, simpler water and heat management, and better tolerance to fuel impurities, leading to higher overall system efficiencies [1]. However, state-of-the-art high temperature PEMFCs suffer from leakage problems associated with liquid electrolytes, such as $\text{H}_3\text{PO}_4$ and protic ionic liquids.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
Authors: Luo, J. (Ekstern), Ali, D. (Intern), Pan, C. (Intern), Li, Q. (Intern)
Pages: 179-179
Publication date: 2016

Host publication information
Title of host publication: ISPE-XV, Uppsala 15-19th August 2016
Article number: P56
Main Research Area: Technical/natural sciences
Electronic versions:
Protic_Organic_Ionic_Plastic_Crystals.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Ptychographic X-ray computed tomography of extended colloidal networks in food emulsions

As a main structural level in colloidal food materials, extended colloidal networks are important for texture and rheology. By obtaining the 3D microstructure of the network, macroscopic mechanical properties of the material can be inferred. However, this approach is hampered by the lack of suitable non-destructive 3D imaging techniques with submicron resolution. We present results of quantitative ptychographic X-ray computed tomography applied to a palm kernel oil based oil-in-water emulsion. The measurements were carried out at ambient pressure and temperature. The 3D structure of the extended colloidal network of fat globules was obtained with a resolution of around 300 nm. Through image analysis of the network structure, the fat globule size distribution was computed and compared to previous findings. In further support, the reconstructed electron density values were within 4% of reference values.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, University of Copenhagen, Paul Scherrer Institut
Authors: Schou Nielsen, M. (Ekstern), Bøgelund Munk, M. (Ekstern), Diaz, A. (Ekstern), Pedersen, E. B. L. (Intern), Holler, M. (Ekstern), Bruns, S. (Ekstern), Risbo, J. (Ekstern), Mortensen, K. (Ekstern), Feidenhans'l, R. K. (Ekstern)
Number of pages: 8
Pages: 21-28
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Food Structure
Volume: 7
ISSN (Print): 2213-3291
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.07 SNIP 1.105 CiteScore 2.45
Quantitative review of degradation and lifetime of solid oxide cells and stacks
A comprehensive review of degradation and lifetime for solid oxide cells and stacks has been conducted. Based on more than 50 parameters from 150 publications and 1,000,000 hours of accumulated testing, this paper presents a quantitative analysis of the current international status of degradation and lifetime in the field. The data is used to visualize specific trends regarding choice of materials, operating conditions and degradation rates. The average degradation rate reported is decreasing and is quickly approaching official targets. The database is published online for open-access and a continued updating by the community is encouraged. Furthermore, the commonly reported test parameters and degradation indicators are discussed. The difficulty in standardizing testing due to variations in cell and stack design, materials and intended purpose of the system is acknowledged. A standardization of reporting of long-term single-cell- and stack-tests is proposed.

Quantization of Hall Resistance at the Metallic Interface between an Oxide Insulator and SrTiO$_3$
The two-dimensional metal forming at the interface between an oxide insulator and SrTiO$_3$ provides new opportunities for oxide electronics. However, the quantum Hall effect, one of the most fascinating effects of electrons confined in two dimensions, remains underexplored at these complex oxide heterointerfaces. Here, we report the experimental observation of quantized Hall resistance in a SrTiO$_3$ heterointerface based on the modulation-doped amorphous-LaAlO$_3$/SrTiO$_3$ heterostructure, which exhibits both high electron mobility exceeding 10,000 cm$^2$/V s and low carrier density on the order of $\sim 10^{12}$ cm$^{-2}$. Along with unambiguous Shubnikov-de Haas oscillations, the spacing of the quantized Hall resistance suggests that the interface is comprised of a single quantum well with ten parallel conducting two-dimensional subbands. This provides new insight into the electronic structure of conducting oxide interfaces and represents an important step towards designing and understanding advanced oxide devices.
Quantum and field effects of oxide heterostructures

The interface between two materials can show radically different properties than either of the bulk parent materials. This is not the least true for oxide interfaces, which can display multiple physical functionalities thus making them ideal for the realisation of so-called multi-plexed devices. In these multi-plexed devices, several inputs are translated into several outputs through the multiple physical functionalities. A highly prominent example of such an oxide interface is the one between LaAlO$_3$ and SrTiO$_3$. Although both LaAlO$_3$ and SrTiO$_3$ in the bulk are electrically insulating and non-magnetic, their interface nonetheless shows attractive properties such as metallic conductivity, superconductivity and ferromagnetism. This thesis will provide an extensive review of the literature concerning the interface metal found in LaAlO$_3$/SrTiO$_3$ as well as in other SrTiO$_3$-based heterostructures. Through this review, several open questions will be revealed, which constitute the scientific aims of this thesis. These open questions will subsequently be addressed through the work presented in the articles that were published during the course of this Ph.D. study. In the review of these published articles, the important aspects of sample preparation will initially be covered. Here, the growth of amorphous-LaAlO$_3$ on SrTiO$_3$ will be addressed in a modified pulsed laser deposition setup. This is followed by an investigation of two high-electron mobility interfaces in SrTiO$_3$-based heterostructures. Specifically, these interfaces are the ones between CaZrO$_3$/SrTiO$_3$ and amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. The sample preparation section is ended by outlining a patterning strategy for the high-electron mobility interface at amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. Subsequently, the effects of electrostatic gating are studied in two different SrTiO$_3$-based heterostructures. Here, it is shown that the interface between amorphous-LaAlO$_3$ and SrTiO$_3$ is superconducting with a larger critical transition temperature than that in LaAlO$_3$/SrTiO$_3$. For γ-Al$_2$O$_3$/SrTiO$_3$ it is shown that non-volatile bipolar resistance switching is possible with a gradual tuning of the interface conductivity. Finally, the so-called quantum Hall effect is demonstrated at the interface between amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. The manifestation of the quantum Hall effect reveals that the interface conductivity is comprised of several subbands conducting in parallel. An outlook will be provided at the end of the thesis judging the research as well as development of oxide electronics and multi-plexed devices.

Quantum and field effects of oxide heterostructures

The interface between two materials can show radically different properties than either of the bulk parent materials. This is not the least true for oxide interfaces, which can display multiple physical functionalities thus making them ideal for the realisation of so-called multi-plexed devices. In these multi-plexed devices, several inputs are translated into several outputs through the multiple physical functionalities. A highly prominent example of such an oxide interface is the one between LaAlO$_3$ and SrTiO$_3$. Although both LaAlO$_3$ and SrTiO$_3$ in the bulk are electrically insulating and non-magnetic, their interface nonetheless shows attractive properties such as metallic conductivity, superconductivity and ferromagnetism. This thesis will provide an extensive review of the literature concerning the interface metal found in LaAlO$_3$/SrTiO$_3$ as well as in other SrTiO$_3$-based heterostructures. Through this review, several open questions will be revealed, which constitute the scientific aims of this thesis. These open questions will subsequently be addressed through the work presented in the articles that were published during the course of this Ph.D. study. In the review of these published articles, the important aspects of sample preparation will initially be covered. Here, the growth of amorphous-LaAlO$_3$ on SrTiO$_3$ will be addressed in a modified pulsed laser deposition setup. This is followed by an investigation of two high-electron mobility interfaces in SrTiO$_3$-based heterostructures. Specifically, these interfaces are the ones between CaZrO$_3$/SrTiO$_3$ and amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. The sample preparation section is ended by outlining a patterning strategy for the high-electron mobility interface at amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. Subsequently, the effects of electrostatic gating are studied in two different SrTiO$_3$-based heterostructures. Here, it is shown that the interface between amorphous-LaAlO$_3$ and SrTiO$_3$ is superconducting with a larger critical transition temperature than that in LaAlO$_3$/SrTiO$_3$. For γ-Al$_2$O$_3$/SrTiO$_3$ it is shown that non-volatile bipolar resistance switching is possible with a gradual tuning of the interface conductivity. Finally, the so-called quantum Hall effect is demonstrated at the interface between amorphous-LaAlO$_3$/(La, Sr)MnO$_3$/SrTiO$_3$. The manifestation of the quantum Hall effect reveals that the interface conductivity is comprised of several subbands conducting in parallel. An outlook will be provided at the end of the thesis judging the research as well as development of oxide electronics and multi-plexed devices.
exhibits a flat discharge curve with low over-potentials until the "sudden death" phenomenon which causes the voltage to drop quickly. On the charge side however, this material exhibits significant over-potentials. These high over-potentials are linked with CO2 development which indicates that the cathode material or electrolyte is being decomposed. This is also seen with Thermally reduced Graphene Oxide (TrGO). The graphene based cathode is interesting as it exhibits a high surface area which in turn increases capacity.

Using the additive LiI, functioning as a redox mediator, the discharge curve remains largely unchanged whilst the charge curve exhibits dramatically lower over-potential, throughout the experiment [1][2]. Under certain conditions the chemistry of the battery changes, resulting in a four electron process that produces the reversible discharge product LiOH rather than Li2O2 which is observed without the redox mediator [2]. This results in higher energy densities and ideally higher cyclability due to the lower over-potentials. Using DEMS we have investigated the gas evolved in the process to determine the electron to oxygen ratio using both cathode materials mentioned.

As has been shown with lithium-air batteries the water content affects the morphology of the discharge product[3]. The effect of changing experimental conditions such as varying water content will be reported.
Relaxation of stresses during reduction of anode supported SOFCs

To assess the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. This work reports further details on a newly discovered creep phenomenon, accelerated creep, taking place during the reduction of a Ni-YSZ anode. This relaxes stresses at a much higher rate (~×10^4) than creep during operation. Thus, the phenomenon of accelerated creep during reduction has to be considered both in the production of stacks and in the analysis of the stress field in a stack based on anode supported SOFCs. Accelerated creep has previously been studied in experiments with simultaneous loading and reduction. The hypothesis for the phenomenon centers around a significant softening of the Ni phase, which amongst other should lead to a significant relaxation of internal stresses in the Ni(O)-YSZ microstructure. The internal residual stresses can be anticipated due to the different thermal contractions of the two phases from the sintering temperature to the reduction temperature. It was thus concluded that with the recorded high creep rates, the stresses in a cell at the time of reduction should decrease significantly over minutes. In this work these internal stresses are measured in-situ before and after the reduction by use of X-ray diffraction. This is done by determining the elastic micro-strains (correlating to the stresses), which are assessed from the widening of the Bragg peaks. This enables us to determine the stresses in the different phases locally inside the microstructure of the composite Ni(O)-YSZ anode. Furthermore, the residual stresses have been modeled during cool-down from the reduction temperature. The stresses have been assessed by use of a combination of a 3D microstructural reconstruction by FIB-SEM, a microstructural finite element model and analytical homogenization considerations. A significant decrease of stresses is observed through the reduction as predicted, which partly confirms the hypothesis for the accelerated creep. Also, a significant relaxation of stresses to lower temperatures (~300°C) was also found. This was confirmed by the models, but is however not consistent with previous recorded coefficients of thermal expansion.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Frandsen, H. L. (Intern), Chatzichristodoulou, C. (Intern), Jørgensen, P. S. (Intern), Kwok, K. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 12
Pages: B11-17-B11-23
Publication date: 2016
based on i) La0.6Sr0.4FeO3 (LSF) and CGO and ii) 10Sc1YSZ ((Y2O3)0.01(Sc2O3)0.10(ZrO2)0.89) and MnCo2O4 seem to be promising combinations and results on manufacturing and testing, including long-term results for >1500 h, of these membranes will be presented. The second part of the presentation will focus on module design and application oriented testing. Here first results from integration of OTMs into the slip stream of a biomass gasifier will be shown. Also highlights from the "Highly Efficient Tubular Membranes for Oxy-Combustion (HETMOC)" European FP7 project are included. In this project a proof-of-concept module with 25 one-end closed BCSF (BaxSr1-xCo0.8Fe0.2O3) tubes was designed and tested in a high pressure test stand designed at DTU. To maximize the partial pressure difference across the membrane, high pressure up to 5 bar was applied on the feed side and a vacuum pump was used to lower the pressure on the permeate side. Results on performance and long-term stability as well as problems encountered during the project will be presented.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science

Authors: Kiebach, W. (Intern), Pirou, S. (Intern), Ovtar, S. (Intern), Bjørnetun Haugen, A. (Intern), Hendriksen, P. V. (Intern)

Publication date: 2016

Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochemical Society. Meeting Abstracts (Online)

Volume: MA2016-02

Article number: 2971

ISSN (Print): 2151-2043

Original language: English


Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

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**Revealing the Origin of Activity in Nitrogen-Doped Nanocarbons towards Electrocatalytic Reduction of Carbon Dioxide**

Carbon nanotubes (CNTs) are functionalized with nitrogen atoms for reduction of carbon dioxide (CO₂). The investigation explores the origin of the catalyst's activity and the role of nitrogen chemical states therein. The catalysts show excellent performances, with about 90% current efficiency for CO formation and stability over 60 hours. The Tafel analyses and density functional theory calculations suggest that the reduction of CO₂ proceeds through an initial rate-determining transfer of one electron to CO₂, which leads to the formation of carbon dioxide radical anion (CO₂C). The initial reduction barrier is too high on pristine CNTs, resulting in a very high overpotentials at which the hydrogen evolution reaction dominates over CO₂ reduction. The doped nitrogen atoms stabilize the radical anion, thereby lowering the initial reduction barrier and improving the intrinsic activity. The most efficient nitrogen chemical state for this reaction is quaternary nitrogen, followed by pyridinic and pyrrolic nitrogen.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Proton conductors, Chinese Academy of Sciences, Huaiyin Normal University, University of Messina

Authors: Xu, J. (Ekstern), Kan, Y. (Ekstern), Huang, R. (Ekstern), Zhang, B. (Ekstern), Wang, B. (Ekstern), Wu, K. (Ekstern), Lin, Y. (Ekstern), Sun, X. (Ekstern), Li, Q. (Intern), Centi, G. (Ekstern), Su, D. (Ekstern)

Number of pages: 5

Pages: 1085-1089

Publication date: 2016

Main Research Area: Technical/natural sciences

**Publication information**

Journal: ChemSusChem (Print)

Volume: 9

Issue number: 10

ISSN (Print): 1864-5631

Ratings:

BFI (2018): BFI-level 2

BFI (2017): BFI-level 1

Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 6.7 SJR 2.385 SNIP 1.276

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1
Reversible Decomposition of Secondary Phases in BaO Infiltrated LSM Electrodes—Polarization Effects

In operando Raman spectroscopy is used to study ceramic La_{0.85}Sr_{0.15}MnO_3±δ electrodes infiltrated with BaO. The aim of this work is to clarify why BaO infiltration reduces the polarization resistance in oxygen containing atmospheres. Prior to the in operando experiments, ex situ X-ray diffraction and Raman spectroscopy reveal the formation of a secondary phase, Ba_3Mn_2O_8, on the electrode. During the in operando Raman investigation of the BaO-infiltrated La_{0.85}Sr_{0.15}MnO_3±δ electrodes, experiments are performed at 300 and 500 °C with oxygen partial pressure 0.1 atm and with −1 or +1 V Applied potential. A changing electrode surface is observed during operation as the Ba_3Mn_2O_8 secondary phase decomposes and manganese oxide accumulates on the electrode surface during cathodic polarization. The observed changes are reversible. These results suggest that the formation of Ba_3Mn_2O_8 is responsible for the reduced polarization resistance observed at open Circuit voltage (OCV) in an oxygen containing atmosphere. Furthermore, the results illustrate the dramatic differences between the electrode surface composition at OCV and during cathodic polarization. Overall, the results highlight the dynamic interactions between minor secondary phases and applied potential, a general effect that may be important for the high-performance frequently observed with ceramic electrodes prepared by infiltration.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Imaging and Structural Analysis, Electrofunctional materials, Montana State University
Authors: Traulsen, M. L. (Intern), McIntyre, M. D. (Ekstern), Norrman, K. (Intern), Sanna, S. (Intern), Mogensen, M. B. (Intern), Walker, R. A. (Ekstern)
Reversible Operation of Solid Oxide Cells for Sustainable Fuel Production and Solar/Wind Load-Balancing

The solid oxide electrochemical cell (SOC) is a promising candidate for large-scale energy storage. In electrolysis mode it stores renewable electricity as chemical energy in the form of fuels like hydrogen and hydrocarbons, and the same cell can be operated in the reversedirection to produce electricity from fuels – either previously stored fuels or from an external supply e.g. natural gas or biogas. This reversibility combined with fuel-flexibility is unique among energy storage technologies like closed-system batteries and single-direction electrolyzers. However, few studies have been conducted with focus on fundamentals or applications of bi-directional operation. This presentation will highlight our recent developments in applying reversible SOCs (RSOCs) for renewable energy storage with respect to cell and stack testing, cell and system design, and techno-economic analysis. At the cell level, long-term testing has shown that improved stability can be achieved by reversible operation compared with steady-state electrolysis operation. Further, we have developed novel Ni-free fuel-electrodes that both outperform conventional Ni-based electrodes and do not catalyze carbon deposition, which opens the door to advanced applications of RSOCs that utilize carbonaceous fuels. At the stack level, we have demonstrated operation that follows real-world time-series electricity supply and demand data, considering a 100% renewable energy scenario where wind power is the only power supply. When the wind power supply exceeds demand, the RSOC stack produces syngas via co-electrolysis of CO2 and H2O. Part of the syngas is converted to methanol downstream in the system to meet the demand of transportation vehicles, and the rest is stored for electrical load balancing by conversion back to electricity in fuel cell mode when electricity demand exceeds the wind power supply. At the system level, techno-economic analyses and system designs for different scales and applications have been realized. A simulation of an RSOC system that uses real-world time-series market prices for electricity and natural gas in Denmark to decide when to operate in electrolysis mode (buying electricity and selling methane) or fuel-cell mode (buying gas and selling electricity) shows the advantage of a reversible system and the changing operating profile as the fraction of wind power supply grows. Finally, we discuss the potential for systems with novel chemistries and components to compete with state-of-the-art rechargeable batteries with respect to cost and round-trip efficiency.
Role of Stress Factors on the Adhesion of Interfaces in R2R Fabricated Organic Photovoltaics

The role of the common stress factors such as high temperature, humidity, and UV irradiation on interface adhesion of roll-to-roll fabricated organic photovoltaic (OPV) devices is investigated. The samples range from bare front electrodes to complete devices. It is shown that applying single stress or combinations of stresses onto the samples variably affect the adhesion properties of the different interfaces in the OPV device. It is revealed that while the exposure of the complete devices to the stresses results in the loss of photovoltaic performance, some interfaces in the devices present improved adhesion properties. Depth profiling analysis on the fractured samples reveals interdiffusion of layers in the structure, which results in the increase of adhesion and change of the debond path. It is shown that through diffusion and intermixing of internal interfaces coupled stresses can increase the adhesion of OPV interfaces by over tenfold. The results are additionally compared to the photovoltaic performance of the complete devices.
In this paper, we investigate three diketopyrrolopyrrole (DPP) based small molecular non-fullerene acceptors, namely Ph(DPP)$_3$, Ph(DPP)$_2$, and PhDMe(DPP)$_2$, focusing on molecular geometry effects on the frontier orbital level, light absorption, molecular configuration, electron mobility, thin film morphology, and photovoltaic performance of both spin-coated ITO based and roll coated large area, ITO- and vacuum-free organic solar cells (OSCs). For spin-coated devices based on P3HT as the donor polymer the solar cells gave power conversion efficiencies (PCEs) in the following order for (P3HT:PhDMe(DPP)$_2$, 0.65%) > (P3HT:Ph(DPP)$_2$, 0.48%) > (P3HT:Ph(DPP)$_3$, 0.31%). All devices present an open circuit voltage ($V_{oc}$) higher than 1.0 V. For the roll-coated devices, the PCEs were found to fall in another order and with lower values (P3HT:Ph(DPP)$_3$, 0.54%) > (P3HT:Ph(DPP)$_2$, 0.43%) > (P3HT:PhDMe(DPP)$_2$, 0.04%) and the highest $V_{oc}$ was 0.82 V. Our preliminary results highlight the influence of geometry, structure and processing on the performance of non-fullerene acceptors.
Roll-coating fabrication of flexible organic solar cells: comparison of fullerene and fullerene-free systems

Flexible organic solar cells (OSCs) based on a blend of low-bandgap polymer donor PTB7-TH and nonfullerene small molecule acceptor IEIC were fabricated via a roll-coating process under ambient atmosphere. Both an indium tin oxide (ITO)-free substrate and a flexible ITO substrate were employed in these inverted OSCs. OSCs with flexible ITO and ITO-free substrates exhibited power conversion efficiencies (PCEs) up to 2.26% and 1.79%, respectively, which were comparable to those of the reference devices based on fullerene acceptors under the same conditions. This is the first example for all roll-coating fabrication procedures for flexible OSCs based on non-fullerene acceptors with the PCE exceeding 2%. The fullerene-free OSCs exhibited better dark storage stability than the fullerene-based control devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Peking University
Pages: 1044-1051
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Materials Chemistry A
Volume: 4
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
DOIs:
10.1039/c5ta07357j
Source: PublicationPreSubmission
Source-ID: 119867021
Publication: Research - peer-review › Journal article – Annual report year: 2016

Roll-to-Roll Printed Electronics for Standalone Smart Windows

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Roll_to_Roll_Printed_Electronics.pdf

Bibliographical note
Symposium PM5 : Hierarchical, Hybrid and Roll-to-Roll Manufacturing for Device Applications
Roll-to-roll printed silver nanowires for increased stability of flexible ITO-free organic solar cell modules

We report the use of roll-to-roll printed silver nanowire networks as front electrodes for fully roll-to-roll processed flexible indium-tin-oxide (ITO) free OPV modules. We prepared devices with two types of back electrodes, a simple PEDOT:PSS back electrode and a PEDOT:PSS back electrode with a printed silver grid in order to simultaneously explore the influence of the back electrode structure on the operational stability of the modules that did not include any UV-protection. We subjected the devices to stability testing under a number of protocols recommended by the international summit on OPV stability (ISOS). We explored accelerated ISOS-D-2, ISOS-D-3, ISOS-L-2, ISOS-L-3, ISOS-O-1 and ISOS-O-2 testing protocols and compared the performance to previous reports employing the same testing protocols on devices with PEDOT:PSS instead of the silver nanowires in the front electrode. We find significantly increased operational stability across all ISOS testing protocols over the course of the study and conclude that replacement of PEDOT:PSS in the front electrode with silver nanowires increase operational stability by up to 1000%. The duration of the tests were in the range of 140–360 days. The comparison of front and back electrode stability in this study shows that the modules with silver nanowire front electrodes together with a composite back electrode comprising PEDOT:PSS and a silver grid present the best operational stability.
Ruled-based control of off-grid electrolysis
This work deals with a ruled-based control strategy to produce hydrogen from wind and wave energy in an offshore platform. These renewable energies feed a set of alkaline electrolyzers that produce H2. The proposed control system allows regulating the operation of the electrolyzers, taking into account the energy available and optimizing the performance of the plant. Simulation results obtained are presented, showing correct operation of the platform under this proposed control.

Scandium-doped zinc cadmium oxide as a new stable n-type oxide thermoelectric material
Scandium-doped zinc cadmium oxide (Sc-doped ZnCdO) is proposed as a new n-type oxide thermoelectric material. The material is sintered in air to maintain the oxygen stoichiometry and avoid instability issues. The successful alloying of CdO with ZnO at a molar ratio of 1:9 significantly reduced the thermal conductivity by up to 7-fold at room temperature. By carefully selecting the Sc-dopant concentrations, a high power factor of $7.1 \times 10^{-4}$ W m$^{-1}$ K$^{-2}$ at 1173 K could be obtained. Therefore, the highest ZT $\sim 0.3$ at 1173 K was achieved for the Zn$_{0.9}$Cd$_{0.1}$Sc$_{0.01}$O$_{1.015}$ sample, and it has so far one of the highest ZT values among those reported for ZnO based thermoelectric materials over the temperature range, e.g., its ZT value at 300 K, which is 0.012, is over 1 order of magnitude higher than that of the state-of-the-art nanostructured Al-doped ZnO, which is 0.0013. It suggests that this material is a good candidate for improving the overall conversion efficiencies in oxide thermoelectric modules. Meanwhile, Sc-doped ZnCdO is robust in air at high temperatures, whereas other n-type materials, such as Al-doped ZnO, will experience rapid degradation of their electrical conductivity and ZT.
Screening of materials for OPV - finding the perfect candidate(s)

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Bundgaard, E. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/FnCtxY5DdJo

Bibliographical note
This article is published Open Access as part of the RSC's Gold for Gold initiative, licensed under a Creative Commons Attribution 3.0 Unported Licence.

Self-Assembled Plasmonic Nanoparticles for Organic Photovoltaics

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Self_Assembled_Plasmonic_Nanoparticles.pdf

Bibliographical note
Symposium EM7 : Functional Plasmonics

Self-supported ceramic substrates with directional porosity by mold freeze casting

Self-supported ceramic substrates with directional porosity by mold freeze casting

Manufacture of thin-film ceramic substrates with high permeability and robustness is of high technological interest. In this work thin (green state thickness ∼500 μm) porous yttria-stabilized zirconia self-supported substrates were fabricated by pouring stable colloidal aqueous suspensions in a mold and applying directional freeze casting. Use of optimized
suspension, cryoprotector additive and mold proved to deliver defect free ceramic films with high dimensional control. Microstructure analysis demonstrated the formation of desirable aligned porosity at macro-structural scale and resulted to be highly dependent on colloidal behaviour and freeze casting conditions. Manufactured green films were joined by lamination at room temperature and sintered to obtain symmetrical cells consisting of two porous self-supported substrate electrodes (±420 μm) and dense yttria stabilized zirconia electrolyte (±10 μm).

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, CSIC
Authors: Gurauskis, J. (Intern), Graves, C. R. (Intern), Moreno, R. (Ekstern), Nieto, M. (Ekstern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: European Ceramic Society. Journal
Volume: 37
Issue number: 2
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.392 SNIP 1.945
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.381 SNIP 1.724
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.146 SNIP 1.645
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.22 SNIP 1.76
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.191 SNIP 1.67
Shaping our energy future by electrospinning

Electrospinning is the most versatile technique to design nanofiber materials with numerous applications in the fields of filtration, membranes, catalysts, reinforcement and biomedicals. Using electrospinning, we are able to design a complex structure from a rich variety of materials including polymers, metals, ceramics and composite, with the ability to control composition, morphology and secondary structure and tailor performance and functionality for specific applications. Moreover, with significant improvement in electrospinning equipment design, industrial-scale electrospinning technologies with production rate of several thousands of square meters per day are transforming advanced material research done in our labs into products serving our everyday life.

This talk will show you the power of electrospinning technology with exciting projects that address the sizable challenges in energy devices by electrospinning. The outcomes of these unique nanofibrous structures are significant improvements in electrochemical performance and durability, which bring our sustainable energy technology one step forward.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Zhang, W. (. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Silicon doped InP as an alternative plasmonic material for mid-infrared

Silicon-doped InP is grown on top of semieluxing iron-doped and sulfur-doped InP substrates by metalorganic vapor phase epitaxy (MOVPE), and the growth parameters are adjusted to obtain various free carrier concentrations from $1.05 \times 10^{19}$ cm$^{-3}$ up to $3.28 \times 10^{19}$ cm$^{-3}$. Midinfrared (IR) reflection spectra of the samples with different carrier concentrations are used to retrieve pertaining dielectric functions as the key factor for understanding plasmonic behavior of InP:Si in the mid-IR wavelength range.

General information
State: Published
Organisations: Department of Photonics Engineering, Plasmonics and Metamaterials, Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Nanophotonic Devices, Centre of Excellence for Silicon Photonics for Optical Communications
Authors: Panah, M. E. A. (Intern), Han, L. (Intern), Christensen, D. V. (Intern), Pryds, N. (Intern), Lavrinenko, A. (Intern), Semenova, E. (Intern)
Number of pages: 2
Publication date: 2016
Simulation, design and proof-of-concept of a two-stage continuous hydrothermal flow synthesis reactor for synthesis of functionalized nano-sized inorganic composite materials

Computational fluid dynamics simulations were employed to evaluate several mixer geometries for a novel two-stage continuous hydrothermal flow synthesis reactor. The addition of a second stage holds the promise of allowing the synthesis of functionalized nano-materials as for example core-shell or decorated particles. Based on the simulation results, a reactor system employing a confined jet mixer in the first and a counter-flow mixer in the second stage was designed and built. The two-stage functionality and synthesis capacity is shown on the example of single- and two-stage syntheses of pure and mixed-phase NiO and YSZ particles.
Computational fluid dynamics, Continuous synthesis, Hydrothermal, Nanoparticles, Reactor design, Supercritical water

DOIs: 10.1016/j.supflu.2016.06.008
Source: FindIt
Source-ID: 2305932868
Publication: Research - peer-review › Journal article – Annual report year: 2016

Slot-Die-Coated V₂O₅ as Hole Transport Layer for Flexible Organic Solar Cells and Optoelectronic Devices
Vanadium pentoxide has been proposed as a good alternative hole transport layer for improving device lifetime of organic photovoltaics. The article presents a study on the optimization of slot-die-coated vanadium oxide films produced with a roll coating machine with the aim of achieving scalable organic solar cells and photo-detectors with improved performance. The effect of different diluents on the electrical properties of the vanadium oxide films is investigated, and methodologies for efficient interfacing of the anode are studied. Furthermore, the lifetime of the cells with incorporated vanadium oxide is investigated employing different encapsulation methods. Finally, an application of the manufactured scalable devices in proximity sensors is demonstrated using a 3D-printed scaffold.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 10
Pages: 1494-1503
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 18
Issue number: 8
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.124 SNIP 2.045
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
This research demonstrates a flexible one-pot strategy for fabricating three-dimensional (3D) boron/nitrogen-doped networks of carbon nanotubes (CNTs)/carbon nanosheets "Line-in-Wall" (LIWNB) based on the space-confined template method. In the synthesis, the high rate of freezing step and freeze-dried process enable the CNTs and carbon-heteroatoms sources confined in the limited space of the self-assembled NaCl salts, which are then heat-treated to obtain a B/N-doped network constructed by "Line-in-Wall" type of carbon hybrids. By combining the 3D B/N-doped carbon nanosheets network and CNTs in this unique pattern, the LIW-NB integrates advantages of three aspects: first, the doped heteroatoms enhancing electrochemical properties of carbon matrix; second, the warp-proof nanosheets supplying high specific surface area; and the extracted and embedded CNTs serving as electron conductive paths and reinforcing the whole architecture. As a result, the 3D LIW-NB shows excellent electrochemical properties: as the electrode of supercapacitors, LIW-NB exhibits high specific capacity at different current densities (389 F g⁻¹ at 1 A g⁻¹ and 129 F g⁻¹ at 20 A g⁻¹); as the lithium ion battery anode, it possesses high reversible storage capacity (1165 mAh g⁻¹ at 0.1 A g⁻¹) and stable long cycle performance at high rate (1000 cycles at 2 A g⁻¹).
The conductivity of pure molten KH$_2$PO$_4$ salt and four mixtures with more or less water (KH$_2$PO$_4$-H$_2$O and KH$_2$PO$_4$-KPO$_3$ systems, respectively) were measured at temperatures of 240-320°C and under their own water vapor pressures. Molten KH$_2$PO$_4$ has been proven to be a promising electrolyte for an elevated temperature pressurized water electrolyzer demonstrating high conductivity of ~0.30 S/cm$^{-1}$ at 300°C. The conductivity data are given as polynomial functions of temperature and composition. The melting point of the pure salt under its own water vapor pressure was determined to be ~272°C.
Stability and Polaronic Motion of Self-Trapped Holes in Silver Halides: Insight through DFT plus U Calculations

Polarons and their associated transport properties are a field of great current interest both in chemistry and physics. To further our understanding of these quasi-particles, we have carried out first-principles calculations of self-trapped holes (STHs) in the model compounds AgCl and AgBr, for which extensive experimental information exists. Our calculations confirm that the STH solely stabilizes in AgCl but with a binding energy of only 165 meV, an order of magnitude smaller than that found for the V_{k} center in KCl. Key contributions to this stabilization energy come from the local relaxation along breathing (a_{1g}) and Jahn Teller (e_{g}) modes in the AgCl_{6}^{4-} unit. To study the transfer of the STH among silver sites, we (i) use first-principles calculations to obtain the hopping barrier of the STH to first and second neighbors, involving eight distinct paths, using first-principles and (ii) construct a simple model, based on Slater-Koster parameters, that highlights the similarity of polaron transfer with magnetic superexchange. This allows one understanding of why the movement of STHs to second neighbors is highly enhanced with respect to closer ones. In agreement with experimental data and the model, the present calculations prove the existence of a dominant mechanism of polaronic motion that corresponds to the displacement of the STHs to the next-nearest sites in the <100> direction and a small barrier of 37 meV. This mechanism is dominated by the covalency inside a AgX_{6}^{4-} complex (X:Cl, Br), thus explaining why the STH is not stabilized in AgBr following the increase of covalence due to the Cl -> Br substitution. The present calculations confirm that, similar to 10% of the charge associated with the STH in AgCl is outside the AgCl_{6}^{4-} complex. This fact is behind the differences between optical: and magnetic properties of the STH in AgCl and those observed in KCl:Ag^{2+}.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Cantabria
Authors: Loftager, S. (Intern), Garcia-Fernandez, P. (Ekstern), Aramburu, J. A. (Ekstern), Moreno, M. (Ekstern), García Lastra, J. M. (Intern)
Number of pages: 16
Pages: 8509-8524
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 16
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Stability of MOF-5 in a hydrogen gas environment containing fueling station impurities

Metal-organic frameworks (MOFs) are an emerging class of porous, crystalline materials with potential application as hydrogen storage media in fuel cell vehicles. Unlike lower capacity adsorbents such as zeolites and carbons, some MOFs are expected to degrade due to attack by impurities present in the hydrogen fuel stream. Hydrogen intended for use in fuel cell vehicles should satisfy purity standards, such as those outlined in SAE J2719. This standard limits the concentration of certain species in the fuel stream based primarily on their deleterious effects on PEM fuel cells. However, the impact of these contaminants on MOFs is mostly unknown. In the present study MOF-5 is adopted as a prototypical moisture-sensitive hydrogen storage material. Five “impure” gas mixtures were prepared by introducing low-to-moderate levels (i.e., up to ~200 times greater than the J2719 limit) of selected contaminants (NH₃, H₂S, HCl, H₂O, CO, CO₂, CH₄, O₂, N₂, and He) to pure hydrogen gas. Subsequently, MOF-5 was exposed to these mixtures over hundreds of adsorption/desorption pressure-swing cycles and for extended periods of static exposure. The impact of exposure was assessed by periodically measuring the hydrogen storage capacity of an exposed sample. Hydrogen chloride was observed to be the only impurity that yielded a measurable, albeit small, decrease in hydrogen capacity; no change in H₂ uptake was observed for the other impurities. Post-cycling and post-storage MOF-5 samples were also analyzed using infrared spectroscopy and x-ray diffraction. These analyses reveal slight changes in the spectra for those samples exposed to HCl and NH₃ compared to the pristine material. These measurements suggest that MOF-5 – and likely many other MOFs – exhibit sufficient robustness to withstand prolonged exposure to ‘off-spec’ hydrogen fuel.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan, Ford Motor Company, BASF
Strain development during the phase transition of La(Fe,Mn,Sn)_{13}H_{z}

We use powder X-ray diffraction to evaluate the temperature dependence of the crystalline properties during the magnetic phase transition of La(Fe,Mn,Sn)_{13}H_{z} as a function of the Fe/Mn/Sn ratio. Both the paramagnetic and ferromagnetic phases were observed as peak overlaps in the patterns around the Curie temperature (T_C) occurring continuously in a temperature range of about 5 K around T_C. Using the Williamson-Hall method, we evaluate the strain developing in the crystallites during the transition and find that it is associated with the growth of the paramagnetic phase as the transition occurs. Based on our measurements and microstructure analyses, we propose that cracking during the phase transition is due to or aggravated by the small content of a La-rich phase.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Chemistry, X-ray Crystallography
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Norby, P. (Intern), Ståhl, K. (Intern), Bahl, C. R. H. (Intern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 109
Issue number: 5
Article number: 051902
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.132 SNIP 0.996
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.799 SNIP 1.462 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.149 SNIP 1.652 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.554 SNIP 1.754 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.805 SNIP 1.94 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Magnetocaloric materials (MCM) with a first order phase transition (FOPT) usually exhibit a large, although sharp, isothermal entropy change near their Curie temperature, compared to materials with a second order phase transition (SOPT). Experimental results of applying FOPT materials in recent magnetocaloric refrigerators (MCR) demonstrated the great potential for these materials, but a thorough study on the impact of the moderate adiabatic temperature change and strong temperature dependence of the magnetocaloric effect (MCE) is lacking. Besides, comparing active magnetic regenerators (AMR) using FOPT and SOPT materials is also of fundamental interest. We present modeling results of multi-layer AMRs using FOPT and SOPT materials based on a 1D numerical model. First the impact of isothermal entropy change, adiabatic temperature change and shape factor describing the temperature dependence of the MCE are quantified and analyzed by using artificially built magnetocaloric properties. Then, based on measured magnetocaloric properties of La(Fe,Mn,Si)13H y and Gd, an investigation on how to layer typical FOPT and SOPT materials with different temperature spans is carried out. Moreover, the sensitivity of variation in Curie temperature distribution for both groups of AMRs is investigated. Finally, a concept of mixing FOPT and SOPT materials is studied for improving the stability of layered AMRs with existing materials.
Single crystalline ceria samples with the composition Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ were pre-polarized with ±5 V for up to 300 s using a Pt coated AFM tip as working electrode. The direct contact zone had a diameter of <50 nm. Subsequently, the effect of the polarization on the surface potential of the samples was investigated by mapping the introduced defect gradient and its decay with time using Kelvin probe force microscopy. The generated surface potential gradients were found to have a diameter of up to 1 μm, which is explained by the local ionization of defect associates by the applied high electric field. Measurements were performed at room temperature and 50°C. The polarization behavior of the Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ single crystals was compared to cyclovoltammetry and polarization-relaxation experiments at T ≤ 350°C and in dry air or nitrogen which were performed using a specially suited AFM (Controlled Atmosphere High Temperature Scanning Probe Microscope CAHT-SPM by Semilab).
Study of variables for accelerating lifetime testing of SOFCs

Solid oxide fuel cell (SOFC) applications require lifetimes of several years on the system level. A big challenge is to proof/confirm/demonstrate such exceptionally long lifetimes. Accelerated or compressed testing are possible methods. Activities in this area have been carried out without arriving at a generally accepted result. First accelerated testing approaches were performed under non-steady operation conditions (current cycling, temperature cycling) by different researchers [1, 2]. However, cycling conditions seemed to have no significant impact on degradation mechanisms. Furthermore, tests done at different current load cycling profiles revealed a strong deviation between predicted and measured lifetime [3]. In this study, we present a detailed analysis of durability results for degradation mechanisms of single SOFC components as a function of operating conditions. Electrochemical impedance data is collected and used to de-convolute the individual losses of single SOFC cell components – electrolyte, cathode and anode. The obtained knowledge is adopted to identify operation profiles and appropriate stresses in order to execute appropriate accelerated testing for lifetime investigation of SOFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Subsolidus Phase Relations of the CaO-REOₓ-CuO Systems (RE = Eu, Tb, Dy, Ho, Er, Lu and Sc) at 900 °C in Air

The subsolidus phase relations of the CaO-REOₓ-CuO systems (RE = Eu, Tb, Dy, Ho, Er, Lu and Sc) were investigated in air at 900 °C. The pseudo-ternary sections with RE = Tb, Dy, Ho, Er and Lu have a similar structure. They have in common with the RE = Eu system a solid solution of Ca₀.₈₃₃−ₓREₓCuO₂⁺y composition but the system with RE = Eu differs by the presence of an Eu₂CuO₄ phase instead of RE₂Cu₂O₅ for RE = Tb, Dy, Ho, Er and Lu. In contrast, the CaO-ScO₁.₅-CuO section does not contain a Ca₀.₈₃₃−ₓScₓCuO₂⁺y solid solution and is dominated by the CaSc₂O₄ phase, which has no equivalent in the other systems at 900 °C in air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Grivel, J. (Intern)
Number of pages: 10
Pages: 601-610
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Phase Equilibria and Diffusion
Volume: 37
Issue number: 5
ISSN (Print): 1547-7037
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.487 SNIP 0.724
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.419 SNIP 0.605 CiteScore 0.64
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.444 SNIP 0.903 CiteScore 0.73
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.355 SNIP 0.733 CiteScore 0.47
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.502 SNIP 0.758 CiteScore 0.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.4 SNIP 0.685 CiteScore 0.44
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.663
BFI (2009): BFI-level 1
Superconducting Dy$_{1-x}$(Gd,Yb)$_x$Ba$_2$Cu$_3$O$_7$ thin films made by Chemical Solution Deposition

Dy$_{1-x}$(Gd or Yb)$_x$Ba$_2$Cu$_3$O$_7$ samples were prepared using chemical solution deposition (CSD), based on trifluoroacetate metal-organic decomposition (MOD) methods. X-ray diffraction results demonstrated the formation of the RE123 superconducting phase with a strong in-plane and out-of-plane texture. c-lattice constants were observed to decrease for all samples doped with Gd or Yb. Measurements of the onset critical transition temperature ($T^{onset}_c$) were found to decrease with increasing Yb content, while only minor changes were observed for samples with Gd. Critical current density (Jc) analysis demonstrated that doping with Yb significantly increased the self-field Jc value from 3.8 MA/cm$^2$ to 6.0 MA/cm$^2$ for the pure and 10% Yb doped sample, respectively. In contrast, samples doped with Gd were characterized by the lowest self-field Jc values. Investigation of pinning force mechanisms revealed that the samples in this study were dominated by normal surface pinning.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Quantum Physics and Information Technology
Authors: Opata, Y. A. (Intern), Wulff, A. C. (Intern), Hansen, J. O. B. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
Synthesis and characterization of 2D layered gadolinium-doped cerium oxide (CGO) nanomaterials

By the virtue of versatility in composition, morphology, and structure, two-dimensional (2D) layered nanomaterials have attracted in the last decade huge interest. Such materials, consisting in stacked charged nanosheets intercalated with opposite charged exchangeable anions, are of great potential for the design and fabrication of nanomaterials in many applications. Indeed, the interlayer gallery provides a flexible space to accommodate various sized molecules (e.g. pollutants) and tune specific active sites at the atomic space (e.g. catalyst materials). The interest for 2D layered nanomaterials is also associated with the possibility of obtaining via exfoliation ultra-thin nanosheets with lateral dimensions of hundreds of nanometres and thickness of few nanometres. This unique class of nanomaterials has shown many unprecedented properties mainly originating from the dimensional anisotropy and nano-confinement effects. Herein we propose novel 2D layered ceria based oxides (e.g. CGO) synthesized via the heterogeneous precipitation. CGO...
materials were selected because of their strategic relevance in many technological applications (e.g., catalysis and electrochemical devices). The synthesized CGO layered materials were characterized for their composition, morphology and crystallographic features. The combined experimental results indicated that the layered CGO, with tunable dopant concentration, can be obtained in different morphologies by controlling the synthesis parameters.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Instituto de Pesquisas Energeticas e Nucleares, Universidade Federal do ABC
Authors: Poras Reis de Moraes, L. (Ekstern), Marani, D. (Intern), Esposito, V. (Intern), Zanetti De Florio, D. (Ekstern), Coral Fonseca, F. (Ekstern)
Number of pages: 1
Publication date: 2016
Event:
Main Research Area: Technical/natural sciences

**Synthesis of ligand-free CZTS nanoparticles via a facile hot injection route**

Single-phase, ligand-free Cu2ZnSnS4 (CZTS) nanoparticles that can be dispersed in polar solvents are desirable for thin film solar cell fabrication, since water can be used as the solvent for the nanoparticle ink. In this work, ligand-free nanoparticles were synthesized using a simple hot injection method and the precursor concentration in the reaction medium was tuned to control the final product. The as-synthesized nanoparticles were characterized using various techniques, and were found to have a near-stoichiometric composition and a phase-pure kesterite crystal structure. No secondary phases were detected with Raman spectroscopy or scanning transmission electron microscopy energy dispersive x-ray spectroscopy. Furthermore, high resolution transmission electron microscopy showed large-sized nanoparticles with an average diameter of 23 nm ± 11 nm. This approach avoids all organic materials and toxic solvents that otherwise could hinder grain growth and limit the deposition techniques. In addition the synthesis route presented here results in nanoparticles of a large size compared to other ligand-free CZTS nanoparticles, due to the high boiling point of the solvents selected. Large particle size in CZTS nanoparticle solar cells may lead to a promising device performance. The results obtained demonstrate the suitability of the synthesized nanoparticles for application in low cost thin film solar cells.

**General information**

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Nanyang Technological University
Authors: Mirbagheri, N. (Intern), Engberg, S. L. J. (Intern), Crovetto, A. (Intern), Simonsen, S. B. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences
Synthesis of Polybenzimidazoles

General information
Systematic Study of Durability of High Temperature PEM Fuel Cells at Selected Temperatures, Flow Rates and Loads

Techniques for PBI Membrane Characterization
Temperature Dependence of Charge Localization in High-Mobility, Solution-Crystallized Small Molecule Semiconductors Studied by Charge Modulation Spectroscopy

In solution-processable small molecule semiconductors, the extent of charge carrier wavefunction localization induced by dynamic disorder can be probed spectroscopically as a function of temperature using charge modulation spectroscopy (CMS). Here, it is shown based on combined field-effect transistor and CMS measurements as a function of temperature that in certain molecular semiconductors, such as solution-processible pentacene, charge carriers become trapped at low temperatures in environments in which the charges become highly localized on individual molecules, while in some other molecules the charge carrier wavefunction can retain a degree of delocalization similar to what is present at room temperature. The experimental approach sheds new insight into the nature of shallow charge traps in these materials and allows identifying molecular systems in which intrinsic transport properties could, in principle, be observed at low temperatures if other transport bottlenecks associated with grain boundaries or contacts could be removed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of Cambridge, Merck Chemicals Ltd., Norwegian University of Science and Technology
Authors: Meneau, A. Y. B. (Ekstern), Olivier, Y. (Ekstern), Backlund, T. (Ekstern), James, M. (Ekstern), Breiby, D. W. (Ekstern), Andreasen, J. W. (Intern), Sirringhaus, H. (Ekstern)
Pages: 2326–2333
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 26
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Original language: English
Electronic versions: Temperature_Dependence_of_Charge_Localization.pdf
The 2016 oxide electronic materials and oxide interfaces roadmap

Oxide electronic materials provide a plethora of possible applications and offer ample opportunity for scientists to probe into some of the exciting and intriguing phenomena exhibited by oxide systems and oxide interfaces. In addition to the already diverse spectrum of properties, the nanoscale form of oxides provides a new dimension of hitherto unknown phenomena due to the increased surface-to-volume ratio. Oxide electronic materials are becoming increasingly important in a wide range of applications including transparent electronics, optoelectronics, magnetoelectronics, photonics, spintronics, thermoelectrics, piezoelectrics, power harvesting, hydrogen storage and environmental waste management. Synthesis and fabrication of these materials, as well as processing into particular device structures to suit a specific application is still a challenge. Further, characterization of these materials to understand the tunability of their properties and the novel properties that evolve due to their nanostructured nature is another facet of the challenge. The research related to the oxide electronic field is at an impressionable stage, and this has motivated us to contribute with a roadmap on 'oxide electronic materials and oxide interfaces'. This roadmap envisages the potential applications of oxide materials in cutting edge technologies and focuses on the necessary advances required to implement these materials, including both conventional and novel techniques for the synthesis, characterization, processing and fabrication of nanostructured oxides and oxide-based devices. The contents of this roadmap will highlight the functional and correlated properties of oxides in bulk, nano, thin film, multilayer and heterostructure forms, as well as the theoretical considerations behind both present and future applications in many technologically important areas as pointed out by Venkatesan. The contributions in this roadmap span several thematic groups which are represented by the following authors: novel field effect transistors and bipolar devices by Fortunato, Grundmann, Boschker, Rao, and Rogers; energy conversion and saving by Zaban, Weidenkaff, and Murakami; new opportunities of photonics by Pompeyrine, and Zuniga-Perez; multiferroic materials including novel phenomena by Ramesh, Spaldin, Mertig, Lorenz, Srinivasan, and Prellier; and concepts for topological oxide electronics by Kawasaki, Pentcheva, and Gegenwart. Finally, Miletto Granozio presents the European action 'towards oxide-based electronics' which develops an oxide electronics roadmap with emphasis on future nonvolatile memories and the required technologies. In summary, we do hope that this oxide roadmap appears as an interesting up-to-date snapshot on one of the most exciting and active areas of solid state physics, materials science, and chemistry, which even after many years of very successful development shows in short intervals novel insights and achievements. Guest editors: M S Ramachandra Rao and Michael Lorenz.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Leipzig, Indian Institute of Technology, Madras, National University of Singapore, Universidade Nova de Lisboa, Qingdao University
Number of pages: 53
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Volume: 49
Issue number: 43
Article number: 433001
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.645 SNIP 0.917
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.693 SNIP 1.046 CiteScore 2.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.069 SNIP 1.383 CiteScore 2.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.18 SNIP 1.469 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.244 SNIP 1.394 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.257 SNIP 1.399 CiteScore 2.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.291 SNIP 1.288
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.283 SNIP 1.337
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.446 SNIP 1.563
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.385 SNIP 1.633
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.203 SNIP 1.466
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.123 SNIP 1.442
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.9 SNIP 1.2
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.99 SNIP 1.221
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.901 SNIP 1.205
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.79 SNIP 1.133
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.925 SNIP 1.249
Original language: English
Oxides, Interfaces, Materials, Oxide electronics
La2-xCoTiO6-delta/Ce0.9Gd0.1O2-delta composites are presented as promising new cathodes for solid oxide fuel cells. The B-site ordering characteristic of double perovskites is present in the whole series. Additionally, increasing amounts of La-vacancies give rise to ordering of alternating La-rich and square-rich (square = vacancy) Layers perpendicular to the c-axis. The introduction of La vacancies produces both oxidation of Co2+ to Co3+ and oxygen vacancies inducing a change of both electrical and electrochemical properties. The best electrochemical performances are obtained for Low x due to a compromise between sufficiently high amount of defects to provide electronic and ionic conductivities, but not so high to induce defect clustering. The material with x = 0.05 exhibits the best performances of the series. Symmetrical cells made of composites of this material and Ce0.9Gd0.1O2-delta deposited on pellets of this electrolyte show a polarization resistance of 0.39 Omega cm(2) at 1073 K.
The effect of tape casting operational parameters on the quality of adjacentely graded ceramic film

For small length tape casting of ceramic slurries varying green film thickness is often a problem. To optimise this, the following parameters were investigated: single blade, double blade, using a pump system and a modelled speed change mode have been analysed. Advantages and limitations of every method are described here. The tape casting experiments were built to be generic in order to allow the control of various processing conditions. From these results, the single-blade technique was chosen for a study of side-by-side tape casting. The influence of the geometric parameters of partitioning the casting tank into chambers, on the quality of graded tape was studied. Tape casting experiments at different speeds and partition tongue lengths in combination with rheological tests revealed that high casting speeds and absence of the partition under the blade are detrimental to the formation of the smooth well-controlled interface between the co-cast slurries, required for most of applications.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Electrofunctional materials
Authors: Bulatova, R. (Intern), Gudik-Sørensen, M. (Intern), Della Negra, M. (Intern), Andersen, K. B. (Intern), Kaiser, A. (Intern), Bahl, C. (Intern)
Number of pages: 9
Pages: 4663-4671
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Ceramics International
Volume: 42
Issue number: 4
ISSN (Print): 0272-8842
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.853 SNIP 1.304
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.846 SNIP 1.299 CiteScore 2.64
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.871 SNIP 1.668 CiteScore 2.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.812 SNIP 1.563 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.816 SNIP 1.766 CiteScore 2.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.922 SNIP 1.758 CiteScore 2.1
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.86 SNIP 1.299
The Impact of Strong Cathodic Polarization on SOC Electrolyte Materials

One of the most promising reversible energy conversion/storage technologies is that of Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC). Long term durability is typically required for such devices to become economically feasible, hence considerable amount of work has and is being done on the degradation and long term durability of these systems. When using a SOC in electrolysis mode, it is economically beneficial to operate the cell at high current density, since it increases the fuel production rate. However, several degradation phenomena, such as segregation of impurities at the grain boundaries, electrode poisoning, delamination or cracks of the electrolyte etc., have been observed in cells operated at such conditions, lowering the lifetime of the cell\(^1\). High polarizations are observed at the electrolyte/cathode interface of an electrolysis cell operated at high current density. In case of a cell voltage above 1.6 V, p-type and n-type electronic conductivity are often observed at the anode and cathode respectively\(^3\). Hence, a considerable part of the current is lost as leakage through the electrolyte, thus lowering the efficiency of the cell considerably.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Fundamental Electrochemistry
Authors: Kreka, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern), Normann, K. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2863
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/39/2863.abstract?sid=4fd302d7-8e22-4be5-bab5-9d8e60878c29

Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016
The Influence of Conjugated Polymer Side Chain Manipulation on the Efficiency and Stability of Polymer Solar Cells

The stability of polymer solar cells (PSCs) can be influenced by the introduction of particular moieties on the conjugated polymer side chains. In this study, two series of donor-acceptor copolymers, based on bis(thiényl)dialkoxybenzene donor and benzo[c][1,2,5]thiadiazole (BT) or thiazolo[5,4-d]thiazole (TzTz) acceptor units, were selected toward effective device scalability by roll-coating. The influence of the partial exchange (5% or 10%) of the solubilizing 2-hexyldecyloxy by alternative 2-phenylethoxy groups on efficiency and stability was investigated. With an increasing 2-phenylethoxy ratio, a decrease in solar cell efficiency was observed for the BT-based series, whereas the efficiencies for the devices based on the TzTz polymers remained approximately the same. The photochemical degradation rate for PSCs based on the TzTz polymers decreased with an increasing 2-phenylethoxy ratio. Lifetime studies under constant sun irradiance showed a diminishing initial degradation rate for the BT-based devices upon including the alternative side chains, whereas the (more stable) TzTz-based devices degraded at a faster rate from the start of the experiment upon partly exchanging the side chains. No clear trends in the degradation behavior, linked to the copolymer structural changes, could be established at this point, evidencing the complex interplay of events determining PSCs’ lifetime.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Department of Chemistry, Hasselt University, Vrije Universiteit Brussel
Authors: Heckler, I. M. (Intern), Kesters, J. (Ekstern), Defour, M. (Ekstern), Madsen, M. V. (Intern), Penxten, H. (Ekstern), D’Haen, J. (Ekstern), Van Mele, B. (Ekstern), Maes, W. (Ekstern), Bundgaard, E. (Intern)
Number of pages: 18
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Materials
Volume: 9
Article number: 181
ISSN (Print): 1996-1944
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 3.26 SJR 0.834 SNIP 1.497
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.852 SNIP 1.495 CiteScore 3.11
Scopus rating (2014): SJR 0.777 SNIP 1.256 CiteScore 2.69
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.998 SNIP 1.673 CiteScore 3.12
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 0.838 SNIP 1.471
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.65 SNIP 1.239
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.394 SNIP 0.99
Original language: English
Conjugated polymers, Side chain variation, Organic photovoltaics, Roll-coating, Photochemical and thermal stability

Electronic versions:
The_Influence.pdf
DOIs:
10.3390/ma9030181
Source: PublicationPreSubmission
Source-ID: 123475097
Publication: Research - peer-review › Journal article – Annual report year: 2016

The lifetime cost of a magnetic refrigerator
The total cost of a 25 W average load magnetic refrigerator using commercial grade Gd is calculated using a numerical model. The price of magnetocaloric material, magnet material and cost of operation are considered, and all influence the total cost. The lowest combined total cost with a device lifetime of 15 years is found to be in the range $150-$400 depending on the price of the magnetocaloric and magnet material. The cost of the magnet is largest, followed closely by the cost of operation, while the cost of the magnetocaloric material is almost negligible. For the lowest cost device, the optimal magnetic field is about 1.4 T, the particle size is 0.23 mm, the length of the regenerator is 40-50 mm and the utilization is about 0.2, for all device lifetimes and material and magnet prices, while the operating frequency vary as function of device lifetime. The considered performance characteristics are based on the performance of a conventional A

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+++ refrigeration unit. In a rough life time cost comparison between the AMR device and such a unit we find similar costs, the AMR being slightly cheaper, assuming the cost of the magnet can be recuperated at end of life.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Bahl, C. R. (Intern), Nielsen, K. K. (Intern)
Number of pages: 22
Pages: 48–62
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Refrigeration
Volume: 63
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.309 SNIP 1.737
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.841 SNIP 1.646
Scopus rating (2006): SJR 1.5 SNIP 1.629
Scopus rating (2005): SJR 1.409 SNIP 1.718
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.193 SNIP 1.933
Scopus rating (2003): SJR 1.241 SNIP 1.542
The magnetic properties of the hollow cylindrical ideal remanence magnet

We consider the magnetic properties of the hollow cylindrical ideal remanence magnet. This magnet is the cylindrical permanent magnet that generates a uniform field in the cylinder bore, using the least amount of magnetic energy to do so. The remanence distribution of this magnet is derived and the generated field is compared to that of a Halbach cylinder of equal dimensions. The ideal remanence magnet is shown in most cases to generate a significantly lower field than the equivalent Halbach cylinder, although the field is generated with higher efficiency. The most efficient Halbach cylinder is shown to generate a field exactly twice as large as the equivalent ideal remanence magnet.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern)
Number of pages: 4
Pages: 321-324
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 416
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285 CiteScore 1.84
Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid

The electrochemical reduction (electroreduction) of CO2 to formic acid (HCOOH) and its competing reactions, that is, the electroreduction of CO2 to CO and the hydrogen evolution reaction (HER), on twenty-seven different metal surfaces have been investigated using density functional theory (DFT) calculations. Owing to a strong linear correlation between the free energies of COOH* and H*, it seems highly unlikely that the electroreduction of CO2 to HCOOH via the COOH* intermediate occurs without a large fraction of the current going to HER. On the other hand, the selective electroreduction of CO2 to HCOOH seems plausible if the reaction occurs via the HCOO* intermediate, as there is little correlation between the free energies of HCOO* and H*. Lead and silver surfaces are found to be the most promising monometallic catalysts showing high faradaic efficiencies for the electroreduction of CO2 to HCOOH with small overpotentials. Our methodology is widely applicable, not only to metal surfaces, but also to other classes of materials enabling the computational search for electrocatalysts for CO2 reduction to HCOOH.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Stanford University, SLAC National Accelerator Laboratory
Authors: Yoo, J. (Ekstern), Christensen, R. (Intern), Vegge, T. (Intern), Nørskov, J. (Ekstern), Studt, F. (Ekstern)
Number of pages: 7
Pages: 358 – 363
Publication date: 2016
Main Research Area: Technical/natural sciences
Theoretical Limiting Potentials in Mg/O₂ Batteries

A rechargeable battery based on a multivalent Mg/O₂ couple is an attractive chemistry due to its high theoretical energy density and potential for low cost. Nevertheless, metal-air batteries based on alkaline earth anodes have received limited attention and generally exhibit modest performance. In addition, many fundamental aspects of this system remain poorly understood, such as the reaction mechanisms associated with discharge and charging. The present study aims to close this knowledge gap and thereby accelerate the development of Mg/O₂ batteries by employing first-principles calculations to characterize electrochemical processes on the surfaces of likely discharge products, MgO and MgO₂. Thermodynamic
limiting potentials for charge and discharge are calculated for several scenarios, including variations in surface stoichiometry and the presence/absence of intermediate species in the reaction pathway. The calculations indicate that pathways involving oxygen intermediates are preferred, as they generally result in higher discharge and lower charging voltages. In agreement with recent experiments, cells that discharge to MgO exhibit low round-trip efficiencies, which are rationalized by the presence of large thermodynamic overvoltages. In contrast, MgO2-based cells are predicted to be much more efficient: superoxide-terminated facets on MgO2 crystallites enable low overvoltages and round-trip efficiencies approaching 90%. These data suggest that the performance of Mg/O2 batteries can be dramatically improved by biasing discharge toward the formation of MgO2 rather than MgO.
We present flexible organic power transistors prepared by fast (20 m/min) roll-to-roll (R2R) flexographic printing[1] of the drain (D) and source (S) electrode structures directly on polyester foil. The devices have top gate architecture and were completed by spin coating or slot-die coating of the organic semiconductor poly-3-hexylthiophene (P3HT) and the dielectric material polystyrene (PVP) before the gate (G) was applied by either screen printing or evaporation of silver. We explore the footprint and the practically accessible geometry of such devices with a special view toward being able to drive large currents while handling the thermal aspects in operation together with other organic printed electronics technologies such as large area organic photovoltaics (OPV)[2] and large area electrochromic displays (EC).[3] We find especially that an elevated operational temperature is beneficial with respect to both transconductance and on/off ratio. We achieve high currents of up to 45 mA at a temperature of 80 °C with an on/off ratio of 100 which is sufficient to drive large area organic electronics such as an EC device powered by OPV devices that we also demonstrate. Finally, we observe a significant temperature dependence of the performance which can be explored further in sensing applications.

The Organic Power Transistor: Roll-to-Roll Manufacture, Thermal Behavior, and Power Handling When Driving Printed Electronics

We present flexible organic power transistors prepared by fast (20 m/min) roll-to-roll (R2R) flexographic printing[1] of the drain (D) and source (S) electrode structures directly on polyester foil. The devices have top gate architecture and were completed by spin coating or slot-die coating of the organic semiconductor poly-3-hexylthiophene (P3HT) and the dielectric material polystyrene (PVP) before the gate (G) was applied by either screen printing or evaporation of silver. We explore the footprint and the practically accessible geometry of such devices with a special view toward being able to drive large currents while handling the thermal aspects in operation together with other organic printed electronics technologies such as large area organic photovoltaics (OPV)[2] and large area electrochromic displays (EC).[3] We find especially that an elevated operational temperature is beneficial with respect to both transconductance and on/off ratio. We achieve high currents of up to 45 mA at a temperature of 80 °C with an on/off ratio of 100 which is sufficient to drive large area organic electronics such as an EC device powered by OPV devices that we also demonstrate. Finally, we observe a significant temperature dependence of the performance which can be explored further in sensing applications.
Thermal analysis of CZTS nanoparticles and inks

General information
State: Published
Organisations: Department of Photonics Engineering, Department of Energy Conversion and Storage, Mixed Conductors, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Optical Microsensors and Micromaterials, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Agersted, K. (Ekstern), Crovetto, A. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Publication date: 2016
Event: Poster session presented at 2016 E-MRS Spring Meeting and Exhibit, Lille, France.
Thermal decomposition of heavy rare-earth butanoates, Ln(C₃H₇CO₂)₃ (Ln = Er, Tm, Yb and Lu) in argon

The thermal behaviour of Ln(C₃H₇CO₂)₃ (Ln = Er, Tm, Yb or Lu) was studied in argon from room temperature by means of thermogravimetry and differential thermal analysis up to 1400 °C, by infrared spectroscopy, hot-stage optical microscopy and X-ray diffraction. Melting prior to decomposition was observed in all four compounds, but its course depends on the rare-earth element. Decomposition to sesquioxides proceeds via the formation of dioxyomono-carbonates (Ln₂O₂CO₃) and release of 4-heptanone (C₃H₇COC₃H₇) as well as carbon dioxide (CO₂) without evidence for an intermediate oxobutanoate stage. During the decomposition of Ln₂O₂CO₃ into the respective sesquioxides (Ln₂O₃), an intermediate plateau extending from approximately 550 to 850 °C appears in the TG traces. The overall composition during this stage corresponds approximately to Ln₂O₂.₈(CO₃)₀.₂, but the state is more probably a mixture of Ln₂O₂CO₃ and Ln₂O₃. The stability of this intermediate state seems to decrease with the mass of the rare-earth elements. Complete conversion to Ln₂O₃ is reached at about 1100 °C. The overall thermal decomposition behaviour of the title compounds is different from previous reports for other rare-earth butanoates.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Hamburg
Authors: Grivel, J. (Intern), Yue, Z. (Intern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Watenphul, A. (Ekstern)
Number of pages: 12
Pages: 1111–1122
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Thermal Analysis and Calorimetry
Volume: 126
Issue number: 3
ISSN (Print): 1388-6150
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.599 SNIP 0.965 CiteScore 1.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.599 SNIP 0.986 CiteScore 1.69
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.641 SNIP 1.189 CiteScore 1.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.458 SNIP 1.277 CiteScore 1.97
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.596 SNIP 1.252 CiteScore 1.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.529 SNIP 1.042 CiteScore 1.55
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.472 SNIP 1.059
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.525 SNIP 1.069
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Thermal decomposition of Yttrium(III) isovalerate in argon

The thermal behaviour of yttrium(III) isovalerate \( \text{Y(C}_{4}\text{H}_{9}\text{CO}_{2})_{3} \) was studied in argon by means of thermogravimetry, differential thermal analysis, FTIR-spectroscopy, hot-stage optical microscopy and X-ray diffraction with a laboratory Cu-tube source as well as with a synchrotron radiation source. Two structural transitions take place in the solid state at 100 °C and 140 °C. They are followed by the decomposition of the isovalerate salt with release of gaseous products consisting of \( \text{CO}_{2} \) and 2,6-dimethyl-4-heptanone and formation of \( \text{Y}_{2}\text{O}_{2}\text{CO}_{3} \) between 320 °C and 440 °C. Above 440 °C, \( \text{Y}_{2}\text{O}_{2}\text{CO}_{3} \) is slowly converted to \( \text{Y}_{2}\text{O}_{3} \) with release of \( \text{CO}_{2} \). The decomposition is complete at about 900 °C.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Yue, Z. (Intern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Watenphul, A. (Ekstern), von Zimmermann, M. (Ekstern)
Number of pages: 6
Pages: 341-346
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Analytical and Applied Pyrolysis
Volume: 120
ISSN (Print): 0165-2370
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.11 SJR 1.353 SNIP 1.533
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.497 SNIP 1.63 CiteScore 4.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.714 SNIP 1.967 CiteScore 4.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.046 SNIP 1.948 CiteScore 3.6
Thermo-Chemo-Mechanical Response of Solid Oxide Cells during Reduction and Cooling

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Amminex Emissions Technology A/S
Authors: Chatzichristodoulou, C. (Intern), Charlas, B. (Ekstern), Kwok, K. (Intern), Jørgensen, P. S. (Intern), Norby, P. (Intern), Hendriksen, P. V. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-01
Article number: 1495
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
Thermo_Chemo_Mechanical.pdf
Links:
http://ma.ecsdl.org/content/MA2016-01/30/1495.abstract
Source: PublicationPreSubmission
Source-ID: 2305368805
Publication: Research - peer-review > Journal article – Annual report year: 2016

Yttrium isovalerate, Thermal decomposition, TG-DTA, FTIR, Carboxylates

DOIs:
10.1016/j.jaap.2016.06.001
Source: FindIt
Source-ID: 2305368805
Publication: Research - peer-review > Journal article – Annual report year: 2016
Thermodynamic modeling of the Sr-Co-Fe-O system

This paper reviews and assesses phase equilibria and thermodynamic properties of phases in the Sr-Co-Fe-O system, with a focus on oxides, especially the SrCo$_{1-x}$Fe$_x$O$_{3-\delta}$ perovskite. In our work, the SrCo$_{1-x}$Fe$_x$O$_{3-\delta}$ perovskite was modeled with a three-sublattice model, where the three sublattices correspond to the A, B and oxygen sites in an ABO$_3$ perovskite, respectively. A number of other important ternary oxide phases in Sr-Co-O and Sr-Co-Fe-O were also considered. Available thermodynamic and phase diagram data were carefully assessed. A thermodynamic description of Sr-Co-O was derived using the CALPHAD approach and was further extrapolated to that of Sr-Co-Fe-O. The thermodynamic database of Sr-Co-Fe-O established in this work allows for calculating phase diagrams, thermodynamic properties, cation distribution and defect chemistry properties, and therefore enables material composition optimization for various applications, including solid oxide fuel cells and oxygen membranes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, Vienna University of Technology
Authors: Zhang, W. W. (Intern), Povoden-Karadeniz, E. (Ekstern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 10
Pages: 88-97
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 292
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.055 SNIP 1.258 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.383 SNIP 1.621 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.459 SNIP 1.503
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.507 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Thermoelectric Properties of Solution-Processed n-Doped Ladder-Type Conducting Polymers

Ladder-type "torsion-free" conducting polymers (e.g., polybenzimidazobenzophenanthroline (BBL)) can outperform "structurally distorted" donor-acceptor polymers (e.g., P(NDI2OD-T2)), in terms of conductivity and thermoelectric power factor. The polaron delocalization length is larger in BBL than in P(NDI2OD-T2), resulting in a higher measured polaron mobility. Structure-function relationships are drawn, setting material-design guidelines for the next generation of conducting thermoelectric polymers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linkoping University, Max-Planck-Institut fur Kohlenforschung
Number of pages: 8
Pages: 10764–10771
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Materials
Volume: 28
Issue number: 48
ISSN (Print): 0935-9648
Ratings:
BFI (2018): BFI-level 3
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 17.79
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
This paper presents a constitutive thermoviscoelastic model for thin films of linear low-density polyethylene subject to strains up to yielding. The model is based on the free volume theory of nonlinear thermoviscoelasticity, extended to orthotropic membranes. An ingredient of the present approach is that the experimentally inaccessible out-of-plane material properties are determined by fitting the model predictions to the measured nonlinear behavior of the film. Creep tests, uniaxial tension tests, and biaxial bubble tests are used to determine the material parameters. The model has been validated experimentally, against data obtained from uniaxial tension tests and biaxial cylindrical tests at a wide range of temperatures and strain rates spanning two orders of magnitude.
The role of hydrogen bonds in the melting points of sulfonate-based protic organic salts

There are three main types of interactions inside organic salts - electrostatic interaction, hydrogen bonding and van der Waals force [1-4]. While van der Waals force is relatively weak, it is hydrogen bonding and particularly electrostatic interaction that determine the lattice energies of ionic systems and other physicochemical properties like melting points [5]. The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation [6]. Hydrogen bonds in the solid state fall into the classification of strong, moderate, and weak hydrogen bonds [7]. In molecular systems like H2O (vs. H2S) or NH3 (vs. PH3), strong hydrogen bonds lead to higher melting points. However, in organic salts, the situation may be different [8,9].
Thin films for energy conversion and storage devices: status and perspective

State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Stamate, E. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
Thin_films_for_energy.pdf

Bibliographical note
Invited lecture
Source: PublicationPreSubmission
Source-ID: 128141809
Publication: Research › Conference abstract for conference – Annual report year: 2016

Three-dimensional numerical modeling of an induction heated injection molding tool with flow visualization

Using elevated mold temperature is known to have a positive influence on final injection molded parts. Induction heating is a method that allow obtaining a rapid thermal cycle, so the overall molding cycle time is not increased. In the present research work, an integrated multi-turn induction heating coil has been developed and assembled into an injection molding tool provided with a glass window, so the effect of induction heating can directly be captured by a high speed camera. In addition, thermocouples and pressure sensors are also installed, and together with the high speed videos, comparison of the induction heating and filling of the cavity is compared and validated with simulations. Two polymer materials ABS and HVPC were utilized during the injection molding experiments carried out in this work. A nonlinear electromagnetic model was employed to establish an effective linear magnetic permeability. The three-dimensional transient thermal field of the mold cavity was then calculated and compared with the experiments. This thermal field was transferred to an injection molding flow solver to compare simulations and experimental results from the high speed video, both with and without the effect of induction heating. A rapid thermal cycle was proved to be feasible in a mold with an integrated induction coil. Furthermore, it was shown that the process can be modeled with good accuracy, both in terms of the thermal field and of the flow pattern.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Guerrier, P. (Intern), Tosello, G. (Intern), Nielsen, K. K. (Intern), Hattel, J. H. (Intern)
Number of pages: 18
Pages: 643-660
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Advanced Manufacturing Technology
Volume: 85
Issue number: 1
Tracking Electronic Pathways in Energy Materials by Low Voltage Scanning Electron Microscopy

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Thydén, K. T. S. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at SCANDEM 2016, Trondheim, Norway.
Main Research Area: Technical/natural sciences
Electronic versions:
- Scandem_2016_poster_jabe_b15K_rev.pdf
- Source: PublicationPreSubmission
- Source-ID: 124915513

Tracking Electronic Pathways in Energy Materials by Low Voltage Scanning Electron Microscopy

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Thydén, K. T. S. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
- SCANDEM2016_poster_abstract_jabe_thyd_4.pdf
- Source: PublicationPreSubmission
- Source-ID: 124915494

Transparent and low emissivity coatings based on aluminum doped zinc oxide

**General information**
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Stamate, E. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 4th International Workshop on Solution Plasma and Molecular Technologies, Pilsen, Czech Republic.
Main Research Area: Technical/natural sciences
Electronic versions:
- Transparent_and_low_emissivity.pdf
- Source: PublicationPreSubmission
- Source-ID: 128141847

Tubular asymmetric oxygen transport membranes

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Bjørnetun Haugen, A. (Intern), Ovtar, S. (Intern), Gurauskis, J. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 6th International Conference on Shaping of Advanced Ceramics, Montpellier, France.
Main Research Area: Technical/natural sciences
Tuning the activity of Pt alloy electrocatalysts by means of the lanthanide contraction

The high platinum loadings required to compensate for the slow kinetics of the oxygen reduction reaction (ORR) impede the widespread uptake of low-temperature fuel cells in automotive vehicles. We have studied the ORR on eight platinum (Pt)–lanthanide and Pt-alkaline earth electrodes, Pt5M, where M is lanthanum, cerium, samarium, gadolinium, terbium, dysprosium, thulium, or calcium. The materials are among the most active polycrystalline Pt-based catalysts reported, presenting activity enhancement by a factor of 3 to 6 over Pt. The active phase consists of a Pt overlayer formed by acid leaching. The ORR activity versus the bulk lattice parameter follows a high peaked “volcano” relation. We demonstrate how the lanthanide contraction can be used to control strain effects and tune the activity, stability, and reactivity of these materials.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Center for Atomic-scale Materials Design, Theoretical Atomic-scale Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Number of pages: 4
Pages: 73-76
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 352
Issue number: 6281
ISSN (Print): 0036-8075
Ratings:
BFI (2018): BFI-level 3
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 12.012 SNIP 8.269 CiteScore 12.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 12.305 SNIP 7.87 CiteScore 12.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 13.159 SNIP 8.124 CiteScore 12.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 14.049 SNIP 8.309 CiteScore 11.97
Understanding degradation of solid oxide electrolysis cells through modeling of electrochemical potential profiles

Establishing the spatial distribution of the various chemical and electrochemical potentials in an operating SOEC is critical as several degradation mechanisms are tightly connected to them, but at the same time very challenging to achieve experimentally. Such distributions are presented here on the basis of a two dimensional bi-layer electrolyte SOC model including for both electrodes a description of activation, concentration, and conversion losses. An extensive parametric study is reported to illustrate the influence of the electrode polarization resistances, the ionic and electronic conductivities in the electrolyte, the gas composition, temperature, and pressure on the current density distribution over the cell and the oxygen activity distribution within the electrolyte. The developed model is further used to simulate long-term durability experiments during different stages of operation, thereby helping to rationalize microstructural and chemical changes observed in post-mortem analysis. Finally, measures to mitigate degradation by changing conditions of operation, material or electrode properties or overall cell geometry are suggested.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors, Department of Chemistry
Authors: Chatzichristodoulou, C. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern), Jacobsen, T. (Intern), Mogensen, M. B. (Intern)
Number of pages: 18
Pages: 265-282
Publication date: 2016
Main Research Area: Technical/natural sciences
bi-layer electrolyte, degradation, electrochemical potential profiles, modeling, SOEC

DOIs:
10.1016/j.electacta.2015.12.067

Source: Findit
Source-ID: 2289880746
Publication: Research - peer-review › Journal article – Annual report year: 2016

Understanding ternary poly(potassium benzimidazolide)-based polymer electrolytes
Poly(2,20-(m-phenylene)-5,50-bisbenzimidazole) (m-PBI) can dissolve large amounts of aqueous electrolytes to give materials with extraordinary high ion conductivity and the practical applicability has been demonstrated repeatedly in fuel cells, water electrolyzers and as anion conducting component in fuel cell catalyst layers. This work focuses on the chemistry of m-PBI in aqueous potassium hydroxide. Equilibration in aqueous KOH with concentrations of 15e20 wt.% was found to result in ionization of the polymer, causing released intermolecular hydrogen bonding. This allowed for extensive volume swelling, high electrolyte uptake, dramatic plasticization and increase of the ion conductivity for the formed poly(potassium benzimidazolide)-based structure. Further increasing the concentration of the bulk solution to 50 wt.% resulted in dehydration and extensive crystallization of the polymer matrix as evidenced by X-ray diffraction, increased density and enhanced elastic modulus. © 2016 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Jankova Atanasova, K. (Intern), Han, J. (Intern), Bjerrum, N. J. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 7
Pages: 304-310
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Polymer
Volume: 84
ISSN (Print): 0032-3861
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.77 SJR 1.191 SNIP 1.252
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.157 SNIP 1.286 CiteScore 3.72
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.321 SNIP 1.619 CiteScore 3.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.415 SNIP 1.666 CiteScore 4.07
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.591 SNIP 1.8 CiteScore 3.74
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.623 SNIP 1.82 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.851 SNIP 1.8
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.999 SNIP 1.72
This paper presents direct and indirect methods for studying the elastocaloric effect (eCE) in shape memory materials and its comparison. The eCE can be characterized by the adiabatic temperature change or the isothermal entropy change (both as a function of applied stress/strain). To get these quantities, the evaluation of the eCE can be done using either direct methods, where one measures (adiabatic) temperature changes or indirect methods where one can measure the stress–strain–temperature characteristics of the materials and from these deduce the adiabatic temperature and isothermal entropy changes. The former can be done using the basic thermodynamic relations, i.e. Maxwell relation and Clausius–Clapeyron equation. This paper further presents basic thermodynamic properties of shape memory materials, such as the adiabatic temperature change, isothermal entropy change and total entropy–temperature diagrams (all as a function of temperature and applied stress/strain) of two groups of materials (Ni–Ti and Cu–Zn–Al alloys) obtained using indirect methods through phenomenological modelling and Maxwell relation. In the last part of the paper, the basic definition of the efficiency of the elastocaloric thermodynamic cycle (coefficient of performance) is defined and discussed.
Universality in Nonaqueous Alkali Oxygen Reduction on Metal Surfaces: Implications for Li−O2 and Na−O2 Batteries

Nonaqueous metal–oxygen batteries, particularly lithium–oxygen and sodium–oxygen, have emerged as possible high energy density alternatives to Li-ion batteries that could address the limited driving range issues faced by electric vehicles. Many fundamental questions remain unanswered, including the origin of the differences in the discharge product formed, i.e., Li2O2 versus Li2O in Li−O2 batteries and NaO2 versus Na2O2 in Na−O2 batteries. In this Letter, we analyze the role of the electrode (electrocatalyst) in determining the selectivity of the discharge product through a tuning of the nucleation overpotential for a given electrolyte. On the basis of a thermodynamic analysis using density functional theory calculations, we demonstrate that the free energy of adsorbed LiO2* is a descriptor determining the nucleation overpotential for the formation of lithium peroxide, Li2O2, the primary discharge product in Li−O2 batteries. Our analysis suggests that Au(100), Ag(111), and Au(111) are capable of nucleating Li2O2 with very low overpotentials. We also show that the free energy of adsorbed NaO2* is a descriptor determining the nucleation rate for sodium superoxide, NaO2, the primary discharge product in Na−O2 batteries. We explore trends in selectivity between 2e− and 4e− oxygen reduction for nucleating Li2O2 and Li2O, respectively, and show that to a first approximation, the selectivity can be determined by a single descriptor, the free energy of adsorbed LiO2*. This is due to the existence of linear scaling between LiO2* and LiO* similar to that observed for OOH* and OH* for aqueous oxygen reduction. This analysis shows that for all materials that possess low nucleation overpotentials, the nucleation overpotential for 2e− oxygen reduction is smaller than that for the 4e− oxygen reduction. In the case of Na−O2, we find that the trends in selectivity between nucleating NaO2 and Na2O2 are determined by the free energy of adsorbed NaO2* and the reorganization energy associated with sodium-ion coupled electron transfer. This analysis provides a rational basis for the selection of the electrode (electrocatalyst) for tuning the nucleation and thereby potentially controlling the discharge product.

Voltage and Thermally Driven High Current RolltoRoll Printed Transistors

Voltage and Thermally Driven High Current RolltoRoll Printed Transistors
Water vapor pressure over molten KH$_2$PO$_4$ and demonstration of water electrolysis at ∼300°C

A new potentially high-efficiency electrolyte for water electrolysis: molten monobasic potassium phosphate, KH$_2$PO$_4$ or KDP has been investigated at temperatures ∼275–325 °C. At these temperatures, KH$_2$PO$_4$ was found to dissociate into H$_2$O gas in equilibrium with a melt mixture of KH$_2$PO$_4$—K$_2$H$_2$P$_2$O$_7$—KPO$_3$—H$_2$O. The water vapor pressure above the melt, when contained in a closed ampoule, was determined quantitatively vs. temperature by use of Raman spectroscopy with methane or hydrogen gas as an internal calibration standard, using newly established relative ratios of Raman scattering cross sections of water and methane or hydrogen to be 0.40 ± 0.02 or 1.2 ± 0.03. At equilibrium the vapor pressure was much lower than the vapor pressure above liquid water at the same temperature. Electrolysis was realized by passing current through closed ampoules (vacuum sealed quartz glass electrolysis cells with platinum electrodes and the electrolyte melt). The formation of mixtures of hydrogen and oxygen gases as well as the water vapor was detected by Raman spectroscopy. In this way it was demonstrated that water is present in the new electrolyte: molten KH$_2$PO$_4$ can be split by electrolysis via the reaction 2H$_2$O → 2H$_2$ + O$_2$ at temperatures ∼275–325 °C. At these temperatures, before the start of the electrolysis, the KH$_2$PO$_4$ melt gives off H$_2$O gas that pressurizes the cell according to the following dissociations: 2KH$_2$PO$_4$ ↔ K$_2$H$_2$P$_2$O$_7$ + H$_2$O ↔ 2KPO$_3$ + 2H$_2$O. The spectra show however that the water by virtue of hydrogen-bonding has a high affinity for remaining in the melt. The formed hydrogen and oxygen gasses were detected by means of the characteristic Raman gas-phase spectra.
Which Electrode Materials to Select for More Environmentally Friendly Organic Photovoltaics?

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Espinosa Martinez, N. (Intern), Laurent, A. (Intern), Benatto, G. A. D. R. (Intern), Hösel, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 6
Pages: 490-495
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Engineering Materials
Volume: 18
Issue number: 4
ISSN (Print): 1438-1656
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.826 SNIP 1.083
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.807 SNIP 1.045 CiteScore 1.82
Web of Science (2015): Indexed yes
In this paper, the feasibility of combined heat and power waste-to-energy plant is investigated in the conditions of implementation of the new legal framework for waste disposal and management as well as new power market conditions. As waste management is a core issue of sustainable development of regions, especially urban and metropolitan areas, as well as a need for sustainable energy supply, these two energy flows logically come together in the facility for heat and power production by waste incineration. However, when new legislation guidelines are implemented, quantity and quality of municipal solid waste as fuel changes, which has a great influence on the operation of waste-to-energy based systems. While there is a lot of fuel in the first years of operation, the feasibility of facilities may come in jeopardy with further development of waste management system. This paper investigates gradual compensation of decreasing municipal solid waste production by introducing new fuels such as woody biomass from the industry, agriculture and energy crops. Scenarios are developed to offer an assessment of the rate of waste replacement with biomass from the surrounding area, taking into account various types of fuel mix with inherent lower heating value changes and sustainability of fuel transport to the plant gate. Due to legislative changes, facility needs to achieve profitability within the energy market and conditions of market trade of energy. Results of the economic analysis show that decreasing waste quantities compensation with woody biomass can increase the feasibility of such projects. In the case of meeting legislation goals by source separation, such
compensation increases the profitability of already profitable projects which enables reduction of gate fees by 32% for same economic results. Further interventions in the waste management system, which include the introduction of the mechanical-biological treatment facility, further reduce the profitability of these kinds of projects and make the viability of this project dependent on fuel compensation.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, University of Zagreb, International Centre for Sustainable Development of Energy, Water and Environment Systems
Authors: Tomić, T. (Ekstern), Dominkovic, D. F. (Intern), Pfeifer, A. (Ekstern), Schneider, D. (Ekstern)
Pages: 165-165
Publication date: 2016

Host publication information
Title of host publication: Book of Abstracts : 11th Conference on Sustainable Development of Energy, Water and Environment Systems
Article number: SDEWES.SEE2016.0088
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Zero carbon energy system of South East Europe in 2050
South East Europe is the region in a part of Europe with approximately 65.5 million inhabitants, making up 8.9% of Europe's total population. The countries concerned have distinct geographical features, various climates and significant differences in gross domestic product per capita, so the integration of their energy systems is considered to be a challenging task. Large differences between energy mixes, still largely dominated by fossil-fuel consumption, make this task even more demanding. This paper presents the transition steps to a 100% renewable energy system which need to be carried out until the year 2050 in order to achieve zero carbon energy society. Novelty of this paper compared to other papers with similar research goals is the assumed sustainable use of biomass in the 100% renewable energy system of the region considered. It is important to emphasize here that only the sustainable use of biomass can be considered carbon-neutral. The resulting biomass consumption of the model was 725.94 PJ for the entire region, which is in line with the biomass potential of the region. Modelling the zero-carbon energy system was carried out using the smart energy system concept, together with its main integration pillars, i.e. power-to-heat and power-to-gas technologies. The resulting power generation mix shows that a wide variety of energy sources need to be utilized and no single energy source has more than a 30% share, which also increases the security of supply. Wind turbines and photovoltaics are the main technologies with shares of 28.9% and 22.5%, followed by hydro power, concentrated solar power, biomass (mainly used in cogeneration units) and geothermal energy sources. To keep the biomass consumption within the sustainability limits, there is a need for some type of synthetic fuel in the transportation sector. Nevertheless, achieving 100% renewable energy system also promises to be financially beneficial, as the total calculated annual socio-economic cost of the region is approximately 20 billion euros lower in the year 2050 than in the base year. Finally, energy efficiency measures will play an important role in the transition to the zero-carbon energy society: the model shows that primary energy supply will be 50.9% lower than in the base year.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalborg University, University of Zagreb, Macedonian Academy of Arts and Science
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Ćosić, B. (Ekstern), Krajačić, G. (Ekstern), Pukšec, T. (Ekstern), Dušić, N. (Ekstern), Markovska, N. (Ekstern)
Number of pages: 12
Pages: 1517–1528
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 184
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Zero carbon energy system of south east europe in 2050 - poster

South East Europe consists of several smaller countries in terms of energy systems and thus, integrating energy systems of the whole region has significant benefits for all the countries included. However, as there are large differences between energy mixes of the countries included, careful energy planning needs to be carried out in order to satisfy energy needs of all the countries of the region. Due to the significant differences in geography and the climate of different parts of the...
region, many different technologies need to be introduced in order to have optimal, low-carbon energy mix. In this paper, steps toward the 100% renewable energy system (RES) for the year 2050 have been presented. Novelty in this paper, compared to the similar research already being carried out, is the sustainable use of biomass in 100% RES, as this is the only way in which biomass can be considered as carbon-neutral. Smart energy systems’ approach has been used in planning of 100% RES, which considers significant integration of the electrical, heating and gas sectors. Many technologies have been employed in the year 2050, but the major share is put on photovoltaics and wind energy, followed by geothermal, solar thermal, CHPs driven on biomass, hydro power and synthetic fuel technologies. Finally, it was shown that the 100% RES in the year 2050 is cheaper than the reference system, developed for the year 2012.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalborg University, University of Zagreb, Macedonian Academy of Arts and Science
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Ćosić, B. (Ekstern), Krajačić, G. (Ekstern), Pukšec, T. (Ekstern), Đurić, N. (Ekstern), Markovska, N. (Ekstern)
Number of pages: 1
Publication date: 2016

**Zero-Gap Alkaline Water Electrolysis Using Ion-Solvating Polymer Electrolyte Membranes at Reduced KOH Concentrations**

Membranes based on poly(2,2’-(m-phenylene)-5,5-bibenzimidazole) (m-PBI) can dissolve large amounts of aqueous KOH to give electrolyte systems with ion conductivity in a practically useful range. The conductivity of the membrane strongly depends on the concentration of the aqueous KOH phase, reaching about $10^{-1}$ S cm$^{-1}$ or higher in 15-25 wt% KOH. Herein, m-PBI membranes are systematically characterized with respect to performance and short-term stability as electrolyte in a zero-gap alkaline water electrolyzer at different KOH concentrations. Using plain uncatalyzed nickel foam electrodes, the cell based on m-PBI outperforms the cell based on the commercially available state-of-the-art diaphragm and reaches a current density of 1500 mA cm$^{-2}$ at 2.4 V in 20 wt% KOH at 80°C. The cell performance remained stable during two days of operation, though post analysis of the membrane using size exclusion chromatography and spectroscopy reveal evidence of oxidative degradation of the base polymer at KOH concentrations of 15 wt% and higher.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kraglund, M. R. (Intern), Aili, D. (Intern), Jankova Atanasova, K. (Intern), Christensen, E. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 7
Pages: F3125-F3131
Publication date: 2016

**Publication information**

Journal: *Electrochemical Society. Journal*
Volume: 163
Issue number: 11
ISSN (Print): 0013-4651
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
Method for producing and controlling the morphology of metal-oxide nanofiber and/or nanotube catalysts. Disclosed herein is a process for the controlled production of metal-containing nanofibers and/or nanotubes, where the morphology of the nanofibers and/or nanotubes is followed in real time by TEM measurements.

**Publication information**
IPC: D01F 9/08 A1
Patent number: WO2015169786
Date: 12/11/2015
Priority date: 06/05/2014
Priority number: EP20140167202
Original language: English
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2015169786
Publication: Research › Patent – Annual report year: 2016

An active magnetic regenerator device
A rotating active magnetic regenerator (AMR) device comprising two or more regenerator beds, a magnet arrangement and a valve arrangement. The valve arrangement comprises a plurality of valve elements arranged substantially immovably with respect to the regenerator beds along a rotational direction. A cam surface is arranged substantially immovably with respect to the magnet arrangement along the rotational direction, and comprises a plurality of cam elements arranged to cooperate with the valve elements in order to control opening degrees of the valve elements, in accordance with a relative position of the cam elements and the valve elements. Thereby the opening degree of each valve element is controlled in accordance with a relative angular position of the regenerator beds and the magnet arrangement.

**Publication information**
IPC: F25B 21/00 A1
Patent number: WO2015118007
Date: 13 Aug 2015
Priority date: 05/02/2014
Priority number: EP20140154015
Original language: English
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2015118007
Publication: Research › Patent – Annual report year: 2015

Oxygen transport membrane.
The present invention relates to a novel composite oxygen transport membrane as well as its preparation and uses thereof.

**General information**
State: Published
Method for Producing Substrates for Superconducting Layers

There is provided a method for producing a substrate suitable for supporting an elongated superconducting element, wherein one or more elongated strips of masking material are placed on a solid element (202) so as to form one or more exposed elongated areas being delimited on one or two sides by elongated strip of masking material, and placing filling material on the solid element so that each exposed elongated area within the one or more exposed elongated areas is covered by a portion of filling material (318a-c) where each portion of filling material also covers at least a portion of the adjacent elongated strip of masking material and subsequently removing the one or more elongated strips of masking material so as to form one or more corresponding undercut volumes, where each undercut volume within the one or more undercut volumes is formed along a portion of filling material and between the portion of filling material and the solid element. The method may further comprise placing buffer material (640) and or superconducting material (642, 644, 646)) on the substrate, so as to provide a superconducting structure (601) with reduced AC losses.

System for cooling a cabinet

The present disclosure relates to a cooling system comprising an active magnetic regenerator having a cold side and a hot side, a hot side heat exchanger connected to the hot side of the magnetic regenerator, one or more cold side heat exchangers, and a cold store reservoir comprising a volume of heat transfer fluid and connected between said one or more cold side heat exchangers and the cold side of the magnetic regenerator, wherein the cooling system is configured to provide a first flow cycle of said heat transfer fluid between the cold store reservoir, the magnetic regenerator and the hot side heat exchanger adapted to transfer thermal energy from the cold store reservoir to the hot side heat exchanger, and at least a second flow cycle of said heat transfer fluid between the cold store reservoir and said one or more cold side heat exchangers adapted to transfer thermal energy from said one or more cold side heat exchangers to the cold store reservoir.
Searching for electrolytes and electrodes for CO₂ reduction below 300 °C

Electrochemical CO₂ reduction research is driven by the desire to reduce reliance on fossil fuels and lower greenhouse gas emissions. The conversion of CO₂ into fuels and chemicals using energy derived from a renewable source, such as wind or solar, could replace the use of fossil fuels.

This thesis uses the knowledge derived from earlier investigations on electrolysis techniques as the foundation for an exploratory work to find acceptable materials and fabricate an electrochemical cell able to produce hydrocarbons and alcohols directly from reduction of CO₂ and steam. The operating conditions should be between 200 – 300 °C and at elevated pressure in the range of 20 – 30 bar. The temperature range is chosen according to the thermal stability of the hydrocarbons produced by conversion of CO₂. The electrochemical performance of the fabricated cells was evaluated using electrochemical impedance spectroscopy and chronoamperometry, while the gas analysis was carried out via gas chromatography.

The initial part of the study focused on electrolyte materials in order to identify a promising candidate to be implemented in the full cells. Some proton conducting materials, such as Y-doped BaZrO₃-BaCeO₃ solid solutions and K-doped BaZr₁₋ₓYₓO₃₋δ were evaluated. BaCe₀.5Zr₀.4Y₀.1O₃₋δ would have been the best electrolyte candidate because of its low resistivity in high pH₂O (2 · 10⁻³ S/cm) even at temperatures as low as 240 °C. However, the instability in the acidic CO₂ gas atmosphere hinders practical application for carbon dioxide reduction at high pressure. K-doped BaZr₁₋ₓYₓO₃₋δ was successfully synthesized by hydrothermal technique, but the conductivity recorded in high pH₂O and at 240 °C was too low (3 · 10⁻⁵ S/cm) to be considered as a suitable electrolyte.

A literature survey showed that most CO₂ reduction studies were performed in aqueous potassium bicarbonate (KHCO₃) and with a copper metal catalyst. Therefore, it was decided to investigate the electrocatalytic activity of copper foam in aqueous media at ambient conditions for electrochemical reduction of CO₂. The measurements were conducted at Stanford University – Chemical Engineer Department, where it was possible to utilize an experimental setup which ensures high sensitivity for minor products from the CO₂ reduction reaction. Seven products were identified with the copper foam electrode tested to -0.98 V vs. RHE. H₂, formate and CO were the main products observed and in particular the faradaic efficiency of H₂ was ca. 90 %. The highest current density that could be sustained with this setup was about -20 mA/cm². Therefore, it was decided to develop a new cell that could operate at higher current densities, pressures and temperatures.

A foam based CO₂ conversion cell with gas diffusion electrodes and a ceramic porous structure in which the liquid electrolyte is immobilized by capillary forces was developed and tested up to 20 bar and to a maximum temperature of 50 °C. Potassium carbonate was selected as aqueous electrolyte and various concentrations of this electrolyte were immobilized in a ceramic porous matrix at both ambient and elevated temperatures and pressures. Copper and silver metal foams were tested as cathode. Nickel metal foam was chosen as anode. When copper was used as electrocatalyst, a high faradaic efficiency for the evolution of H₂, i.e. between 92 to 99 % was registered. The other products detected were CO and during one test also methane was identified. The performance of Ag cathode metal foam confirmed its higher selectivity for CO₂ reduction to CO. The formation of passive oxide layers and the subsequent degradation of nickel foam electrodes affected the electrochemical performance and the stability of the cells negatively.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Vico, F. (Intern), Mogensen, M. B. (Intern), Chatzichristodoulou, C. (Intern), Holtappels, P. (Intern)
Number of pages: 148
Publication date: May 2015
1,2,4-Triazolium perfluorobutanesulfonate as an archetypal pure protic organic ionic plastic crystal electrolyte for all-solid-state fuel cells

1,2,4-Triazolium perfluorobutanesulfonate (1), a novel, pure protic organic ionic plastic crystal (POIPC) with a wide plastic crystalline phase, has been explored as a proof-of-principle anhydrous proton conductor for all-solid-state high temperature hydrogen/air fuel cells. Its physicochemical properties, including thermal, mechanical, structural, morphological, crystallographic, spectral, and ion-conducting properties, as well as fuel cell performances, have been studied comprehensively in both fundamental and device-oriented aspects. With superior thermal stability, 1 exhibits crystal (phase III), plastic crystalline (phase II and I) and melt phases successively from 173 °C to 200 °C. Differential scanning calorimetry and temperature dependent powder X-ray diffraction (XRD) measurements together with polarized optical microscopy and thermomechanical analysis reveal the two solid–solid phase transitions of 1 at 76.8 °C and 87.2 °C prior to the melting transition at 180.9 °C, showing a wide plastic phase (87–181 °C). Scanning electron microscopy displays the morphology of different phases, indicating the plasticity in phase I. Single-crystal XRD studies reveal the molecular structure of 1 and its three-dimensional N–H/O hydrogen bonding network. The influence of the three-dimensional hydrogen bonding network on the physicochemical properties of 1 has been highlighted. The temperature dependence of hydrogen bonding is investigated by variable-temperature infrared spectroscopy. The sudden weakening of hydrogen bonds at 82 °C seems to be coupled with the onset of orientational or rotational disorder of the ions. The temperature dependence of ionic conductivity in the solid and molten states is measured via impedance spectroscopy and current interruption technique, respectively. The Arrhenius plot of the ionic conductivity assumes a lower plateau region (phase I, 100–155 °C) with a low activation energy of 36.7 kJ mol⁻¹ (i.e. 0.38 eV), suggesting likely a Grothuss mechanism for the proton conduction. Variable-temperature infrared analysis, optical morphological observations, and powder XRD patterns further illustrate the structural changes. Electrochemical hydrogen pumping tests confirm the protonic nature of the ionic conduction observed in the lower plateau region. Finally, measurements of the open circuit voltages (OCVs) and the polarization curves of a dry hydrogen/air fuel cell prove the long-range proton conduction. At 150 °C, a high OCV of 1.05 V is achieved, approaching the theoretical maximum (1.11 V).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, KU Leuven, Carl Von Ossietzky University Oldenburg, Soochow University, Chinese Academy of Sciences, Shanghai Jiao Tong University
Authors: Luo, J. (Ekstern), Jensen, A. H. (Intern), Brooks, N. R. (Ekstern), Sniekers, J. (Ekstern), Knipper, M. (Ekstern), Aili, D. (Intern), Li, Q. (Intern), Vanroy, B. (Ekstern), Wübbenhorst, M. (Ekstern), Yan, F. (Ekstern), Van Meervelt, L. (Ekstern), Shao, Z. (Ekstern), Fang, J. (Ekstern), Luo, Z. (Ekstern), De Vos, D. E. (Ekstern), Binnemans, K. (Ekstern),
Accelerated Degradation for Hardware in the Loop Simulation of Fuel Cell-Gas Turbine Hybrid System
The U.S. Department of Energy (DOE)-National Energy Technology Laboratory (NETL) in Morgantown, WV has developed the hybrid performance (HyPer) project in which a solid oxide fuel cell (SOFC) one-dimensional (1D), real-time operating model is coupled to a gas turbine hardware system by utilizing hardware-in-the-loop simulation. To assess the long-term stability of the SOFC part of the system, electrochemical degradation due to operating conditions such as current density and fuel utilization have been incorporated into the SOFC model and successfully recreated in real time. The mathematical expression for degradation rate was obtained through the analysis of empirical voltage versus time plots for different current densities and fuel utilizations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, U.S. DOE National Energy Technology Laboratory, McMaster University
Accelerated DFT-Based Design of Materials for Ammonia Storage

Future energy carriers are needed in order to lower the CO2 emissions resulting from the burning of fossil fuels. One possible energy carrier is ammonia, which can be stored safely and reversibly in metal halide ammines; however, the release often occurs in multiple steps at too high temperatures. Therefore, there is a need for new materials, releasing the ammonia in a narrow temperature interval. To search for new mixed metal halide chlorides, we use DFT calculations guided by a genetic algorithm (GA) to expedite the search, as the defined search space allowing up to three different metals contains more than 100,000 different structures. Here, we search for materials releasing the ammonia between 0 and 100 °C, a temperature range suitable for system integration with low-temperature polymer electrolyte membrane fuel cells (PEMFC). The efficiency of the implemented algorithm is verified by three trial runs capable of finding the same
optimal mixtures starting from different random populations, testing <5% of the candidates. Some of the best candidates are already confirmed experimentally, and others offer a record high, accessible hydrogen capacity exceeding 9 wt %. Among the identified materials is the first known high-capacity ternary metal halide ammine, which we have subsequently synthesized and confirmed the ammonia storage properties using temperature-programmed desorption (TPD).

**General information**

State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Technical University of Denmark, Amminex Emissions Technology A/S
Number of pages: 10
Pages: 4552–4561
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Chemistry of Materials
Volume: 27
Issue number: 13
ISSN (Print): 0897-4756
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 8.89 SJR 4.114 SNIP 1.905
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 4.038 SNIP 2.102 CiteScore 9.38
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 3.603 SNIP 2.253 CiteScore 8.89
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 3.658 SNIP 2.277 CiteScore 8.94
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 4.169 SNIP 2.264 CiteScore 8.1
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 3.484 SNIP 2.145 CiteScore 7.38
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 3.267 SNIP 1.849
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 2.894 SNIP 1.763
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 2.882 SNIP 1.844
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 3.111 SNIP 1.863
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 3.168 SNIP 1.943
Accelerated testing of solid oxide fuel cell stacks for micro combined heat and power application

State-of-the-art (SoA) solid oxide fuel cell (SOFC) stacks are tested using profiles relevant for use in micro combined heat and power (CHP) units. Such applications are characterised by dynamic load profiles. In order to shorten the needed testing time and to investigate potential acceleration of degradation, the profiles are executed faster than required for real applications. Operation with fast load cycling, both using hydrogen and methane/steam as fuels, does not accelerate degradation compared to constant operation, which demonstrates the maturity of SoA stacks and enables transferring knowledge from testing at constant conditions to dynamic operation. 7.5 times more cycles than required for 80,000 h lifetime as micro CHP are achieved on one-cell-stack level. The results also suggest that degradation mechanisms that proceed on a longer time-scale, such as creep, might have a more dominating effect for long life-times than regular short time changes of operation. In order to address lifetime testing it is suggested to build a testing program consisting of defined modules that represent different application profiles, such as one module at constant conditions, followed by modules at one set of dynamic conditions etc.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Hagen, A. (Intern), Høgh, J. V. T. (Intern), Barfod, R. (Ekstern)
Number of pages: 6
Pages: 223-228
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 300
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Acid-base Chemistry and Proton Conductivity of High Temperature Polymer Electrolytes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Li, Q. (Intern), Aili, D. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2015

Bibliographical note
Financial support by the Danish Energy Authority EUDP in the project: Test Center for Fuel Cell and Hydrogen Technologies. Phase 1. (EUDP 09-II, 64009-0246)

Relations
Projects:
Accelerated testing of solid oxide fuel cell stacks for micro combined heat and power application
Source: FindIt
Source-ID: 2281836518
Publication: Research - peer-review › Journal article – Annual report year: 2015
Acido-basic control of the thermoelectric properties of poly(3,4-ethylenedioxythiophene)tosylate (PEDOT-Tos) thin films

PEDOT-Tos is one of the conducting polymers that displays the most promising thermoelectric properties. Until now, it has been utterly difficult to control all the synthesis parameters and the morphology governing the thermoelectric properties. To improve our understanding of this material, we study the variation in the thermoelectric properties by a simple acido-basic treatment. The emphasis of this study is to elucidate the chemical changes induced by acid (HCl) or base (NaOH) treatment in PEDOT-Tos thin films using various spectroscopic and structural techniques. We could identify changes in the nanoscale morphology due to anion exchange between tosylate and Cl- or OH-. But, we identified that changing the pH leads to a tuning of the oxidation level of the polymer, which can explain the changes in thermoelectric properties. Hence, a simple acid-base treatment allows finding the optimum for the power factor in PEDOT-Tos thin films.
Activated Carbon Nanochains with Tailored Micro-Meso Pore Structures and Their Application for Supercapacitors

Carbon nanochains (CNCs) were synthesized by a facile chemical vapor deposition process consisting of a 1D chain of interconnected carbon nano-onions for potential application in supercapacitors. In this study, the CNCs were further activated by a chemical method using potassium hydroxide (KOH) as the activation agent to obtain micro-meso pore structures. To improve the specific surface area (SSA) and optimize the pore size distribution (PSD) to enhance the capacitance performance, we investigated the activation parameters, including the KOH content, temperature and duration. The results indicated that CNCs with a hierarchical pore structure and high SSA could be achieved using an activation process with a KOH-to-CNC ratio of 2 at 900 degrees C for 20 h. The mechanism is also discussed. The activation temperature and duration affect the promotion of the carbon graphitization and exaggeration of the carbon etching. The CNCs activated using the optimal parameters exhibited a high capacitance performance of 112.7 F g(-1) at 50 mV s(-1) with excellent stability in 6 M KOH electrolyte, which was due to the improved surface and micromesoporosity without sacrificing their electronic transmission properties.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tianjin University
Authors: Zhang, M. (Ekstern), He, C. (Ekstern), Liu, E. (Ekstern), Zhu, S. (Ekstern), Shi, C. (Ekstern), Li, J. (Ekstern), Li, Q. (Intern), Zhao, N. (Ekstern)
Number of pages: 8
Pages: 21810-21817
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry C
Volume: 119
Issue number: 38
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Active Cooling and Thermal Management of a Downhole Tool Electronics Section

High Temperature (HT) wellbores represent one of today’s biggest challenges for the oil and gas industry. The majority of well intervention wireline tools contain temperature sensitive electronics that are not able to withstand the high temperatures of HT wellbores (> 150 °C), for an extended period of time. This work presents the design and construction of an actively cooled laboratory prototype, which is able to operate at temperatures which are higher than the temperature limit of the electronics. A different concept of heat management, compared to prior works, is presented: the design combines active and passive cooling techniques, aiming at an efficient thermal management, preserving the tool compactness and avoiding the use of moving parts. Thermoelectric coolers were used to transfer the dissipated heat from the temperature-sensitive electronics to the external environment. Thermal contact resistances were minimized and thermally insulating foam protected the refrigerated microenvironment from the hot surroundings.

A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO2 reduction

Using a DFT-based genetic algorithm (GA) approach, we have determined the most stable structure and stoichiometry of a 309-atom icosahedral AuCu nanoalloy, for potential use as an electrocatalyst for CO2 reduction. The identified core–shell nano-particle consists of a copper core interspersed with gold atoms having only copper neighbors and a gold surface with a few copper atoms in the terraces. We also present an adsorbate-dependent correction scheme, which enables an accurate determination of adsorption energies using a computationally fast, localized LCAO-basis set. These show that it is possible to use the LCAO mode to obtain a realistic estimate of the molecular chemisorption energy for systems where the computation in normal grid mode is not computationally feasible. These corrections are employed when calculating adsorption energies on the Cu, Au and most stable mixed particles. This shows that the mixed Cu135@Au174 core–shell nanoalloy has a similar adsorption energy, for the most favorable site, as a pure gold nanoparticle. Cu, however, has the effect of stabilizing the icosahedral structure because Au particles are easily distorted when adding adsorbates.
Air-processed organic tandem solar cells on glass: toward competitive operating lifetimes

Photovoltaic devices based on organic semiconductors (OPVs) hold great promise as a cost-effective renewable energy platform because they can be processed from solution and deposited on flexible plastics using roll-to-roll processing. Despite important progress and reported power conversion efficiencies of more than 10% the rather limited stability of this type of devices raises concerns towards future commercialization. The tandem concept allows for both absorbing a broader range of the solar spectrum and reducing thermalization losses. We designed an organic tandem solar cell with an inverted device geometry comprising environmentally stable active and charge-selecting layers. Under continuous white light irradiation, we demonstrate an extrapolated, operating lifetime in excess of one decade. We elucidate that for the current generation of organic tandem cells one critical requirement for long operating lifetimes consists of periodic UV light treatment. These results suggest that new material approaches towards UV-resilient active and interfacial layers may enable efficient organic tandem solar cells with lifetimes competitive with traditional inorganic photovoltaics.
Alkali Metal-O₂ Batteries. Performance and Lifetime Limiting Effects

The rechargeable Na-O₂ and Li-O₂ batteries are attractive battery technologies as they potentially are very cheap and as they theoretically possess about 3 and 10 times higher energy density than the current Li-ion technologies. This PhD thesis is dedicated to studying the effects that limit cell performance of these two technologies.

The Li-O₂ battery was first introduced in 1996 and focus in the field is still on understanding the fundamental mechanisms controlling discharge and charge. This PhD thesis was mainly dedicated to the Li-O₂ battery and initially charge conduction through the discharge product, Li₂O₂, was investigated. This was done by using of a conventional three electrode cell in which the heterogeneous electron transfer rate of three different redox couples were studied on Li₂O₂ coated glassy carbon electrodes to provide a measure of the conductivity of the Li₂O₂ layers. Charge transport through Li₂O₂ gives further evidence that hole transport dominates charge-transfer through Li₂O₂. Electrochemical impedance spectroscopy was also used to conduct detailed investigations of surface capacitance, ion transport, and charge-transfer reactions in the cathode of the Li-O₂ cell. The capacitance of the cathode was shown to be sensitive to the thickness of the deposited Li₂O₂ layer. These investigations also explored the influence of the composition of the electrolyte and conditions, which favors a solution mediated Li₂O₂ deposition mechanism. On charge, an electrochemical “safe” operating voltage was identified until 3.30 V were an interface layer was formed, which activates side reactions and further increases the cell potential. A number of ionic liquids were also investigated for their oxygen diffusivity and solubility and while these were in the order of currently employed aprotic electrolytes as the ionic liquids significantly decompose under electrochemical operation. Last, the influence of CO₂ was investigated and it was suggested that CO₂ blocks the step valleys of the deposited Li₂O₂ forcing Li₂O₂ growth away from the electrode surface hereby increasing cell capacity, as the discharge becomes less limited by the cathode surface area.

The Na-O₂ battery is an even newer technology as it was first introduced to the scientific community in 2010. The two batteries are experimentally quite similar as the only difference is the choice of anode. However, when one studies the two systems, the mechanisms controlling each type of battery are quite different. The discharge and charge processes of the non-aqueous Na-O₂ battery were studied in this thesis. On discharge, the deposition mechanism of NaO₂ was shown to be highly dependent on the current density and cell limitations could be correlated to the depositions mechanisms. On charge, three regions of NaO₂ oxidation were identified, each corresponding to a different type of NaO₂ oxidation.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry
Authors: Knudsen, K. B. (Intern), Hjelm, J. (Intern), Jensen, S. H. (Intern), Holtappels, P. (Intern)
Number of pages: 193
Publication date: 2015

Publication information
Place of publication: Kgs. Lyngby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Ambient effects on the electrical conductivity of carbon nanotubes

We show that the electrical conductivity of single walled carbon nanotubes (SWCNT) networks is affected by oxygen and air humidity under ambient conditions by more than a magnitude. Later, we intentionally modified the electrical conductivity by functionalization with iodine and investigated the changes in the band structure by optical absorption spectroscopy. Measuring in parallel the tubes electrical conductivity and optical absorption spectra, we found that conduction mechanism in SWCNT is comparable to that of intrinsically conducting polymers. We identified, in analogy to conducting polymers, in the infrared spectra a new absorption band which is responsible for the increased conductivity, leading to a closing gap in semiconducting SWCNT. We could show that by different functionalizations of the same SWCNT starting material the properties like conductivity can be dramatically changed, leading to different imaginable applications. We investigated here, an ultraviolet sensor with weakly modified SWCNT.
A model for the impact of the nanostructure size on its gas sensing properties

The size of a metal oxide nanostructure plays a key role in its performance as a gas sensor. ZnO nanostructures with different morphologies including nanowires at different diameters and nanodisks at different thicknesses were synthesized hydrothermally. Gas sensors based on individual nanostructures with different sizes were fabricated and their sensing
properties were compared and investigated. Nanowires with smaller diameter size and higher surface to volume ratio showed enhanced gas sensing performance. Also, as the nanodisk thickness gets closer to the thickness of the ZnO depletion layer, the sensitivity increases significantly due to the semi complete depletion of the nanostructure. Our results were explained using a modified general formula for a ZnO ethanol sensor. The formula was established based on the chemical reaction between ethanol molecules and oxygen ions and considering the effect of the surface to volume ratio as well as the depletion region of the nanostructure. This work can be simply generalized for other metal oxides to enhance their performance as gas sensors.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, College of Technological Studies, Public Authority for Applied Education and Training, University of Hail, University of Surrey
Authors: Alenezi, M. R. (Ekstern), Alzanki, T. (Ekstern), Almeshal, A. (Ekstern), Alshammari, A. (Ekstern), Beliatis, M. (Intern), Henley, S. (Ekstern), Silva, S. (Ekstern)
Number of pages: 8
Pages: 103195-103202
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: RSC Advances
Volume: 5
Issue number: 125
ISSN (Print): 2046-2069
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Original language: English
DOIs: 10.1039/c5ra19404k
Source: Findit
Source-ID: 276972153
Publication: Research - peer-review › Journal article – Annual report year: 2015

Analysis of the Interphase on Carbon Black Formed in High Voltage Batteries
Carbon black (CB) additives commonly used to increase the electrical conductivity of electrodes in Li-ion batteries are generally believed to be electrochemically inert additives in cathodes. Decomposition of electrolyte in the surface region of CB in Li-ion cells at high voltages up to 4.9 V is here studied using electrochemical measurements as well as structural and surface characterizations. LiPF\(_6\) and LiClO\(_4\) dissolved in ethylene carbonate:diethylene carbonate (1:1) were used as the electrolyte to study irreversible charge capacity of CB cathodes when cycled between 4.9 V and 2.5 V. Synchrotron-based soft X-ray photoelectron spectroscopy (SOXPES) results revealed spontaneous partial decomposition of the electrolytes on the CB electrode, without applying external current or voltage. Depth profile analysis of the electrolyte/cathode interphase indicated that the concentration of decomposed species is highest at the outermost surface of the CB. It is concluded that carboxylate and carbonate bonds (originating from solvent decomposition) and LiF (when LiPF\(_6\) was used) take part in the formation of the decomposed species. Electrochemical impedance spectroscopy...
measurements and transmission electron microscopy results, however, did not show formation of a dense surface layer on CB particles.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Imaging and Structural Analysis, Uppsala University  
Authors: Younesi, R. (Intern), Christiansen, A. S. (Intern), Scipioni, R. (Intern), Ngo, D. (Intern), Simonsen, S. B. (Intern), Edström, K. (Ekstern), Hjelm, J. (Intern), Norby, P. (Intern)  
Pages: A1289-A1296  
Publication date: 2015  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochemical Society. Journal  
Volume: 162  
Issue number: 7  
ISSN (Print): 0013-4651  
Ratings:  
BFI (2018): BFI-level 1  
BFI (2017): BFI-level 1  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.417 SNIP 1.312  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.45 SNIP 1.267  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.608 SNIP 1.416  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.58 SNIP 1.325  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.611 SNIP 1.54  
Web of Science (2006): Indexed yes  
Scopus rating (2005): SJR 1.519 SNIP 1.484
Analysis of the Interphase on Carbon Black Formed in High Voltage Batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Imaging and Structural Analysis, Uppsala University
Authors: Younesi, R. (Intern), Christiansen, A. S. (Intern), Scipioni, R. (Intern), Ngo, D. (Intern), Simonsen, S. B. (Intern), Edström, K. (Ekstern), Hjelm, J. (Intern), Norby, P. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Analysis_of_the_Interphase.pdf
DOI: 10.1149/2.0761507jes

An efficient numerical scheme for the simulation of parallel-plate active magnetic regenerators
A one-dimensional model of a parallel-plate active magnetic regenerator (AMR) is presented in this work. The model is based on an efficient numerical scheme which has been developed after analysing the heat transfer mechanisms in the regenerator bed. The new finite difference scheme optimally combines explicit and implicit techniques in order to solve the one-dimensional conjugate heat transfer problem in an accurate and fast manner while ensuring energy conservation. The present model has been thoroughly validated against passive regenerator cases with an analytical solution. Compared to the fully implicit scheme, the proposed scheme achieves more accurate results, prevents numerical errors and requires less computational effort. In AMR simulations the new scheme can reduce the computational time by 88%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Universidad Politecnica de Valencia
Authors: Torregrosa-Jaime, B. (Ekstern), Corberán, J. M. (Ekstern), Payá, J. (Ekstern), Engelbrecht, K. (Intern)
Pages: 121-130
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: International Journal of Refrigeration
Volume: 58
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.309 SNIP 1.737
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.841 SNIP 1.646
Scopus rating (2006): SJR 1.5 SNIP 1.629
Scopus rating (2005): SJR 1.409 SNIP 1.718
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.193 SNIP 1.933
Scopus rating (2003): SJR 1.241 SNIP 1.542
Scopus rating (2002): SJR 1.592 SNIP 1.807
Scopus rating (2001): SJR 1.775 SNIP 1.86
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.001 SNIP 1.279
Scopus rating (1999): SJR 0.824 SNIP 1.213
Original language: English
Regenerator, Modelling, Simulation, Magnetic refrigerator, Finite differences
Electronic versions:
Torregrosa_et_al_2015.pdf
DOIs:
10.1016/j.ijrefrig.2015.06.007
An Electrochemical Impedance Spectroscopy Investigation of the Overpotentials in Li−O2 Batteries

Lithium−O2 (Li−O2) batteries are currently limited by a large charge overpotential at practically relevant current densities, and the origin of this overpotential has been heavily debated in the literature. This paper presents a series of electrochemical impedance measurements suggesting that the increase in charge potential is not caused by an increase in the internal resistance. It is proposed that the potential shift is instead dictated by a mixed potential of parasitic reactions and Li2O2 oxidation. The measurements also confirm that the rapid potential loss near the end of discharge (“sudden death”) is explained by an increase in the charge transport resistance. The findings confirm that our theory and conclusions in ref 1, based on experiments on smooth small-area glassy carbon cathodes, are equally valid in real Li−O2 batteries with porous cathodes. The parameter variations performed in this paper are used to develop the understanding of the electrochemical impedance, which will be important for further improvement of the Li−air battery.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, IBM Almaden Research Center, Haldor Topsoe AS
Authors: Højberg, J. (Intern), McCloskey, B. D. (Ekstern), Hjelm, J. (Intern), Vegge, T. (Intern), Johansen, K. (Ekstern), Norby, P. (Intern), Luntz, A. C. (Ekstern)
Pages: 4039−4047
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 7
Issue number: 7
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.571 SNIP 0.931
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Original language: English
Li−O2 batteries, Electrochemical impedance spectroscopy, Overpotential, Mixed potential, Battery performance
DOIs:
An investigation on the role of thermal fins in the design of micro heat exchangers

The different dominant physical phenomena in design for micro and macro scale products result in different design considerations for both categories. In the current study, a few design concepts are proposed as micro heat exchangers. In addition, the influential parameters on design of a micro heat exchanger in comparison with the effective factors in designing its macro counterpart are investigated. Numerical simulations in the finite element software COMSOL are used to evaluate the thermal performance of both micro and macro heat exchangers. The result of the analysis reveals the fact that the presence of some features such as “fins” in micro heat exchanger is not as significant as it is in macro scale. The results of this study can be employed as guidelines in design of similar micro heat exchangers.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Omidvarnia, F. (Intern), Hansen, H. N. (Intern), Sarhadi, A. (Intern)
Number of pages: 2
Publication date: 2015

An isoindigo containing donor-acceptor polymer: synthesis and photovoltaic properties of all-solution-processed ITO- and vacuum-free large area roll-coated single junction and tandem solar cells

In this work, the design, synthesis, and characterization of a donor-acceptor polymer from dithieno[3,2-b:2',3'-d]pyrrole and isoindigo (I-ID) are presented. The synthesized polymer has been applied in large area ITO-free organic photovoltaics, both as spin coated and roll coated devices; the latter as both single junction and multi junction organic photovoltaic (OPV) architectures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Aalborg University, Aarhus University
Number of pages: 7
Pages: 1633-1639
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry C
Volume: 3
ISSN (Print): 2050-7526
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.14 SJR 1.806 SNIP 1.28
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.751 SNIP 1.577 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.505 SNIP 1.36 CiteScore 4.64
Anode Support Creep

Initial reduction temperature of an SOC is kept higher than the highest intended operation temperature of the SOC to keep the electrolyte under compression by the Anode Support at all temperatures equal to and below the maximum intended operation temperature.

A novel CO₂- and SO₂-tolerant dual phase composite membrane for oxygen separation

A novel dual phase composite oxygen membrane (Al₀.₀₂Ga₀.₀₂Zn₀.₉₆O₁.₀₂ - Gd₀.₁Ce₀.₉O₁.₉₅₋δ) was successfully prepared and tested. The membrane shows chemical stability against CO₂ and SO₂, and a stable oxygen permeation over 300 hours in CO₂ was demonstrated. ZnO is cheap and non-toxic and is therefore highly advantageous compared to other common materials used for the purpose.
Assessment of (Mn,Co)$_3$O$_4$ powders for possible coating material for SOFC/SOEC interconnects

In this work (Mn,Co)$_3$O$_4$ spinel powders with different Mn:Co ratio (1:1 and 1:2) and from different commercial suppliers are evaluated for possible powder for production of interconnect coatings. Sinterability of the powders is evaluated on pressed pellets sintered in oxidizing and in reducing/oxidizing atmospheres. For selected powder, coatings are then prepared by the electrophoretic deposition method on Crofer 22 APU stainless steel coupons. Effects of dispersant/iodine content and deposition voltage and times are evaluated. Thickness as a function of deposition parameters is described. Results show that with appropriate powder it is possible to produce adherent protective coating with a well-controlled thickness.
A Study of e⁻ Transport through Li₂O₂, the Main Discharge Product in the Li-O₂ Battery

In the field of energy storage devices the pursuit for cheap, high energy density, reliable secondary batteries is at the top of the agenda. The Li-O2 battery is one of the possible technologies that, in theory, should be able to close the gap, which exists between the present state-of-the-art Li-ion technologies and the demand placed on batteries by technologies such as electrical vehicles [1]. However, the Li-O2 battery still suffers greatly from high overpotentials during oxygen reduction and evolution reactions (discharge and charge, respectively), poor rechargeability, and decomposition of salts and solvents etc. [2] [3]. In order to improve the electrochemical performance of the Li-O2 batteries; it is crucial to understand the fundamental mechanisms that govern and limits the system during electrochemical operation. Here we present a redox probing study of the charge transfer across the deposition product lithium peroxide, Li₂O₂, using outer-sphere redox shuttles: cobaltocene, ferrocene, and decamethylferrocene. The change in heterogeneous electron transfer exchange rate as a function of the potential and the Li₂O₂ layer thickness (~state of charge) was determined using electrochemical impedance spectroscopy. The attenuation of the electron transfer exchange rate with film thickness is dependent on the probing potential, indicating that hole tunneling is the dominant process for charge transfer through Li₂O₂ supporting previous work by Luntz et al. [4]. Additionally, this work includes the determination of diffusion coefficients and concentrations of the redox shuttles and the superoxide ion, in a 1,2-dimethoxyethane based electrolyte. References [1] S. A. Freunberger, P. G. Bruce, L. J. Hardwick et J.-M. Tarascon, «Li-O2 and Li-S batteries with high energy storage,» Nature Materials, vol. 11, pp. 19-29, 2012. [2] B. D. McCloskey, A. Valery, A. C. Luntz, S. R. Gowda, G. M. Wallraff, J. M. Garcia, T. Mori et L. E. Krupp, «Combining Accurate O2 and Li2O2 Assays to Separate Discharge and Charge stability Limitations in Nonaqueous Li-O2 Batteries,» J. Phys. Chem. Lett., vol. 4, pp. 2989-2993, 2013. [3] R. Younesi, M. Hahlin, F. Bjørefors, P. Johansson et K. Edström, «Li-O2 Battery Degradation by Lithium Peroxide (Li2O2): A Model Study,» Chem. Mater., vol. 25, pp. 77-84, 2013. [4] A. C. Luntz, V. Viswanathan, J. Voss, J. B. Varley, J. K. Nørskov, R. Scheffler and A. Speidel, “Tunneling and Polaron Charge Transport through Li2O2 in Li-O2 Batteries,” J. Phys. Chem. Lett., vol. 4,
A study of thermoelectric β-Zn4Sb3 under thermal cycling and large temperature gradients

Band bending and alignment at the spinel/perovskite γ-Al2O3/SrTiO3 heterointerface
Bipolar polaron pair recombination in P3HT/PCBM solar cells

The unique properties of organic semiconductors make them versatile base materials for many applications ranging from light emitting diodes to transistors. The low spin-orbit coupling typical for carbon-based materials and the resulting long spin lifetimes give rise to a large influence of the electron spin on charge transport which can be exploited in spintronic devices or to improve solar cell efficiencies. Magnetic resonance techniques are particularly helpful to elucidate the microscopic structure of paramagnetic states in semiconductors as well as the transport processes they are involved in. However, in organic devices the nature of the dominant spin-dependent processes is still subject to considerable debate. Using multi-frequency pulsed electrically detected magnetic resonance (pEDMR), we show that the spin-dependent response of P3HT/PCBM solar cells at low temperatures is governed by bipolar polaron pair recombination involving the positive and negative polarons in P3HT and PCBM, respectively, thus excluding a unipolar bipolaron formation as the main contribution to the spin-dependent charge transfer in this temperature regime. Moreover the polaron-polaron coupling strength and the recombination times of polaron pairs with parallel and antiparallel spins are determined. Our results demonstrate that the pEDMR pulse sequences recently developed for inorganic semiconductor devices can very successfully be transferred to the study of spin and charge transport in organic semiconductors, in particular when the different polarons can be distinguished spectrally.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technische Universität München
Authors: Kupijai, A. J. (Ekstern), Behringer, K. M. (Ekstern), Corazza, M. (Intern), Gevorgyan, S. (Intern), Krebs, F. C. (Intern), Stutzmann, M. (Ekstern), Brandt, M. S. (Ekstern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: arXiv
Article number: arXiv:1505.01411v1
Original language: English
Electronic versions:
Bipolar_polaron_pair_recombination_in_P3HTPCBM_solar_cells.pdf
Links:
http://arxiv.org/pdf/1505.01411
Publication: Research › Journal article – Annual report year: 2015

Bipolar polaron pair recombination in polymer/fullerene solar cells

We present a study of the rate-limiting spin-dependent charge-transfer processes in different polymer/fullerene bulk-heterojunction solar cells at 10 K. Observing central spin-locking signals in pulsed electrically detected magnetic resonance and an inversion of Rabi oscillations in multifrequency electron-double-resonance spectroscopy, we find that the spin response of both spin-coated and printed P3HT/PCBM and spin-coated PCDTBT/PCBM solar cells at low temperatures is governed by bipolar polaron pair recombination and quantitatively determine the polaron-polaron coupling strength with double electron-electron resonance experiments. Furthermore spin Hahn echo decay and inversion recovery measurements are performed to measure spin coherence and recombination times of the polaron pairs, respectively.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technische Universität München
Authors: Kupijai, A. J. (Ekstern), Behringer, K. M. (Ekstern), Schaeble, F. G. (Ekstern), Galfe, N. E. (Ekstern), Corazza, M. (Intern), Gevorgyan, S. A. (Intern), Krebs, F. C. (Intern), Stutzmann, M. (Ekstern), Brandt, M. S. (Ekstern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences
Capillary based Li-air batteries for in situ synchrotron X-ray powder diffraction studies

For Li-air batteries to reach their full potential as energy storage system, a complete understanding of the conditions and reactions in the battery during operation is needed. To follow the reactions in situ a capillary-based Li-O2 battery has been developed for synchrotron-based in situ X-ray powder diffraction (XRPD). In this article, we present the results for the analysis of 1st and 2nd deep discharge and charge for a cathode being cycled between 2 and 4.6 V. The crystalline precipitation of Li2O2 only is observed in the capillary battery. However, there are indications of side reactions. The Li2O2 diffraction peaks grow with the same rate during charge and the development of the full width at half maximum (FWHM) is hkl dependent. The difference in the FWHM of the 100 and the 102 reflections indicate anisotropic morphology of the Li2O2 crystallites or defects along the c-axis. The effect of constant exposure of X-ray radiation to the electrolyte and cathode during charge of the battery was also investigated. X-ray exposure during charge leads to changes in the development of the intensity and the FWHM of the Li2O2 diffraction peaks. The X-ray diffraction results are supported by ex situ X-ray photoelectron spectroscopy (XPS) of discharged cathodes to illuminate non-crystalline deposited materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Storm, M. M. (Intern), Johnsen, R. E. (Intern), Younesi, R. (Intern), Norby, P. (Intern)
Number of pages: 7
Pages: 3113-3119
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 6
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
Cathodes, Crystalline materials, Electric batteries, Electrodes, Full width at half maximum, Lithium, Lithium batteries, Secondary batteries, X ray diffraction, X ray powder diffraction, Deposited materials, Diffraction peaks, Energy storage systems, In-situ synchrotrons, Li-air batteries, Situ X-ray powder diffraction, X ray radiation, X-ray exposure, X ray photoelectron spectroscopy
Electronic versions:
Capillary_based_Li_air_batteries_for_in_situ_synchrotron_X_ray_powder_diffraction_studies.postprint.pdf. Embargo ended: 16/12/2015
Carbon Deposition during CO2 Electrolysis in Ni-Based Solid-Oxide-Cell Electrodes

Local gradients within an operating solid oxide electrolyzer cell were studied using current-potential measurements and electrochemical impedance spectroscopy. The cells and operating conditions were closely related to commercial applications. The cells with fuel electrodes of nickel and yttria-stabilized zirconia (Ni-YSZ) cermets were supplied by Haldor Topsoe A/S and the operating conditions were chosen so as to take stack relevant considerations into account.

Formation of carbon nanotubes in Ni containing fuel electrodes has previously been observed in co-electrolysis of H2O and CO2 [1]. Hence, the carbon formation threshold in an operating cell was investigated during electrolysis of an idealized reactant atmosphere of CO and CO2. The electrolysis current was gradually increased in steps until the cell voltage spontaneously increased, thereby indicating cell degradation and possibly the onset of carbon deposition. The outlet gas composition at each current step was estimated based on the inlet gas composition and the reactant conversion using Faraday's law. The increase in voltage was observed at lower pCO/pCO2 ratios than that corresponding to the thermodynamic threshold for carbon formation. Electrochemical impedance spectroscopy in both H2/H2O and CO/CO2 revealed an increase in resistance of the fuel electrode after each CO2 electrolysis current-voltage curve, indicating possible carbon deposition. The difference in partial oxygen pressure between inlet and outlet was analyzed to verify carbon deposition. The increase in voltage is likely due to either blocking of the reaction sites by the deposited carbon, or due to the microstructural damage caused by the carbon, or a combination of these.

Moreover, the current step-size and step-length was varied to investigate the time-dependence of the detection of carbon deposition. Initial results indicate that for longer current steps, carbon formation is observed at lower pCO/pCO2 ratios. This is related to the rate of carbon deposition and the averaged nature of the cell voltage measurements. Possible reasons for these observations will be discussed in detail.

In an attempt to mitigate the degradation due to carbon deposition, the Ni-YSZ electrode was infiltrated with a gadolinium doped ceria (CGO) solution. Initial results indicate that the coking tolerance was not enhanced, but it is still unclear whether infiltrated cells degrade less. However, infiltrated cells display a significant performance enhancement before coking, especially under electrolysis current.

The investigation thus indicated carbon formation in the Ni containing fuel electrode before the thermodynamically calculated threshold for average measurements of the cell was reached. The deviation from the average threshold was reproduced on several cells and quantified (figure 1). The observation of carbon formation on a local, microstructural level before the expected thermodynamic threshold for average measurements on the cell level, is of crucial importance when choosing operating conditions for commercial systems. The effect would be even more severe on stack level, where the gas diffusion and temperature gradients are more pronounced. Initial results of the mitigation strategy of infiltrating CGO are negative, but increased performance prior to coking was observed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Skafte, T. L. (Intern), Graves, C. R. (Intern), Blennow, P. (Ekstern), Hjelm, J. (Intern)
Number of pages: 9
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-03
Issue number: 395
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

Carbon Deposition during CO2 Electrolysis in Ni-Based Solid-Oxide-Cell Electrodes
The carbon formation threshold in an operating cell was investigated during electrolysis of an idealized reactant atmosphere of CO and CO2. The electrolysis current was gradually increased in steps until the cell voltage spontaneously increased, thereby indicating cell degradation and possibly the onset of carbon deposition. The outlet gas composition at each current step was estimated based on the inlet gas composition and the reactant conversion using Faraday's law. The increase in voltage was observed at lower outlet pCO/pCO2 ratios than that corresponding to the expected thermodynamic threshold for carbon formation. The degradation observed was related to the fuel electrode, as confirmed by electrochemical impedance spectroscopy. Mitigation of the degradation mechanism was attempted by infiltrating
gadolinium doped ceria. The onset of carbon deposition was largely unaffected, but the polarization resistance of the electrode during electrolysis was significantly decreased.

Carbon Thin-layer Encapsulated Fe-N-C as Active Catalysts for Oxygen Reduction

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Zhong, L. (Intern), Pan, C. (Intern), Hu, Y. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 1
Catalytic Enhancement of Carbon Black and Coal-Fueled Hybrid Direct Carbon Fuel Cells

Hybrid direct carbon fuel cells (HDCFCs) consisting of a solid carbon (carbon black)-molten carbonate (62–38 wt% Li-K)2CO3 mixtures in the anode chamber of an anode-supported solid oxide fuel cell type full-cell are tested for their electrochemical performance between 700 and 800°C. Performance was investigated using current-voltage-power density curves. In the anode chamber, catalysts are mixed with the carbon-carbonate mixture. These catalysts include various manganese oxides (MnO2, Mn2O3, Mn3O4, MnO), metal carbonates (Ag2CO3, MnCO3, Ce2(CO3)3), metals (Ag, Ce, Ni), doped-ceria (CeO2, Ce1-xGdxO2-x/2, Ce1-xREExO2-δ (REE = Pr, Sm)) and metal oxides (LiMn2O4, Ag2O). Materials showing the highest activity in carbon black (Mn2O3, CeO2, Ce0.6Pr0.4O2-δ, Ag2O) were subsequently tested for catalytic activity toward bituminous coal, as revealed by both I-V-P curves and electrochemical impedance spectroscopy (EIS). Catalytic activity was evaluated as a function of various physical characteristics of doped ceria and manganese-based materials.
Catalytic Surface Promotion of Composite Cathodes in Protonic Ceramic Fuel Cells

Composite cathodes based on an electronic conductor and a protonic conductor show advantages for protonic ceramic fuel cells. In this work, the performance of a La$_{5.5}$WO$_{11.25-\delta}$/La$_{0.8}$Sr$_{0.2}$MnO$_{3+\delta}$ (LWO/LSM) composite cathode in a fuel cell based on an LWO protonic conducting electrolyte is shown and catalytically improved. The limiting processes were first unambiguously associated to surface steps, and the reaction rate was significantly enhanced by 1) tailoring the catalytic activity through electrode surface impregnation with intrinsically catalytic nanoparticles and 2) electrochemical activation of surface species by imposing a net current through the electrode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Universidad Politecnica de Valencia
Authors: Solis, C. (Ekstern), Navarrete, L. (Ekstern), Bozza, F. (Intern), Bonanos, N. (Intern), Serra, J. M. (Ekstern)
Pages: 1106-1110
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemElectroChem
Volume: 2
ISSN (Print): 2196-0216
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Chalcogenide compounds made by pulsed laser deposition at 355 and 248 nm

Thin films made by pulsed laser deposition may differ depending on the laser wavelength. We compared ZnS, Cu2SnS3 and a target enriched with SnS relative to Cu2SnS3 using 355 nm and 248 nm lasers.

Characterization of the contact between Bi2Te3-based materials and lead-free solder alloy under thermal cycling

Possible changes in the oxidation state of the oxygen ion in the lithium iron phosphate Li3Fe2(PO4)3 at high voltages in lithium-ion (Li-ion) batteries are studied using experimental and computational analysis. Results obtained from
synchrotron-based hard X-ray photoelectron spectroscopy and density functional theory (DFT) show that the oxidation state of O$_{\delta^-}$ ions is altered to higher oxidation states (O$_{\delta^-}$, $\delta < 2$) upon charging Li$_3$Fe$_2$(PO$_4$)$_3$ to 4.7 V.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry
Number of pages: 4
Pages: 3213-3216
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: ChemSusChem (Print)
Volume: 8
Issue number: 19
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.385 SNIP 1.276
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.494 SNIP 1.411 CiteScore 7.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.863 SNIP 1.663 CiteScore 7.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.548 SNIP 1.452 CiteScore 6.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.046 SNIP 1.563 CiteScore 6.72
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.945 SNIP 1.134
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.973 SNIP 0.72
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.291 SNIP 0.48
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.273 SNIP 0.495
Scopus rating (2006): SJR 0.243 SNIP 0.372
Scopus rating (2005): SJR 0.195 SNIP 0.285
Scopus rating (2004): SJR 0.214 SNIP 0.276
Scopus rating (2003): SJR 0.276 SNIP 0.419
Scopus rating (2002): SJR 0.312 SNIP 0.586
Scopus rating (2001): SJR 0.292 SNIP 0.496
Scopus rating (2000): SJR 0.422 SNIP 0.556
Scopus rating (1999): SJR 0.511 SNIP 0.708

Original language: English
Electronic versions:
Charge Transfer Induced Modulation Doping at Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology, Beijing, China.
Main Research Area: Technical/natural sciences
Electronic versions:
Charge_Transfer.pdf
Source: PublicationPreSubmission
Source-ID: 118749934
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Charge transfer induced modulation doping of two-dimensional electron gas at complex oxide interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern), Trier, F. (Intern), Christensen, D. V. (Intern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from TO-BE Spring Meeting 2015, Aveiro, Portugal.
Main Research Area: Technical/natural sciences
Electronic versions:
Charge_transfer_induced_modulation.pdf
Source: PublicationPreSubmission
Source-ID: 118749873
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Colloidal stabilization of cerium-gadolinium oxide (CGO) suspensions via rheology
A rheological method based on the analysis of the flow index is proposed for the optimization of ceramic suspensions with respect to dispersant-ceramic affinity, dispersant concentration, and ceramic loading. The single-flow index (SFI) feature was identified as the criterion defining the optimized colloidal stable state. The method was applied to explore the ability of four commercial dispersants (acidic affine, neutral, basic affine, and polyvinylpyrrolidone (PVP)) to disperse cerium-gadolinium oxide (CGO) in ethanol. Only the acidic affine and the PVP dispersants were found to efficiently disperse the CGO powder. The acidic affine dispersant was further demonstrated to impart superior packing properties due to the formation of a thinner monolayer around the ceramic surface. CGO suspensions using the acidic affine at optimized amount were prepared and processed via tape casting. The resulting green tapes exhibited uniform and high packing density, producing a theoretical density in the sintered tapes of ca. 97-98%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors
Authors: Marani, D. (Intern), Sudireddy, B. R. (Intern), Bentzen, J. J. (Intern), Jørgensen, P. S. (Intern), Kiebach, R. (Intern)
Pages: 2823–2832
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Comparative Indoor and Outdoor Degradation of Organic Photovoltaic Cells via Inter-laboratory Collaboration

We report on the degradation of organic photovoltaic (OPV) cells in both indoor and outdoor environments. Eight different research groups contributed state of the art OPV cells to be studied at Pomona College. Power conversion efficiency, fill factor, and IV curves were collected at regular intervals over six to eight months. Similarly prepared devices were measured indoors, outdoors, and after dark storage. Device architectures are compared. Cells kept indoors performed better than outdoors due to the lack of temperature and humidity extremes. Encapsulated cells performed better due to the minimal oxidation. Some devices showed steady aging but many failed catastrophically due to corrosion of electrodes not active device layers. Degradation of cells kept in dark storage was minimal over periods up to one year.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Pomona College, Technische Universität Dresden, IMEC, Holst Center, Institut für Solarenergieforschung, Ilmenau University of Technology, Centre d'Investigació en Nanociència i Nanotecnologia, Heliatek GmbH
Number of pages: 4
Pages: 1-4
Publication date: 2015

Host publication information
Title of host publication: Proceedings of 2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC)
Publisher: IEEE
ISBN (Electronic): 978-1-4799-7944-8
Main Research Area: Technical/natural sciences
Conference: 42nd IEEE Photovoltaic Specialists Conference, New Orleans, United States, 14/06/2015 - 14/06/2015
DOIs: 10.1109/PVSC.2015.7356178
Source: FindIt
Source-ID: 276914242
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Comparing superconducting and permanent magnets for magnetic refrigeration

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern), Bahl, C. R. (Intern), Smith, A. (Intern), Wulff, A. C. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-7
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions: E7_DTU_Sustain_2015.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Comparison of direct and indirect plasma oxidation of NO combined with oxidation by catalyst

Direct and indirect plasma oxidation of NOx was tested in a medium-scale test-bench at gas flows of 50 slm (3 m³/h). For direct plasma oxidation the synthetic flue gas was directed through a stacked DBD reactor. For indirect plasma oxidation, a DBD reactor was used to generate ozone from pure O-2 and the plasma treated gas including ozone was
mixed with flue gas at the entrance of a 6 m long serpentine-like reaction chamber which allowed reaction times longer than 10 s. At relatively low NOx concentrations of 200 ppm, both oxidation methods gave similar results. However, the temperature increase of the DBD reactor decreased the long-term efficiency of direct plasma oxidation. At the same time, the efficiency of indirect oxidation increased at elevated reactor temperatures. Additional experiments were carried out to investigate the improvement of indirect oxidation by the introduction of catalyst to the reaction zone. Small-scale experiments with TiO2 powder demonstrated considerable efficiency gain for NOx oxidation while in medium-scale experiments, the efficiency improvement remained negligible. (c) 2014 Elsevier Ltd. All rights reserved.
Comparison Study of YBa$_2$Cu$_3$O$_{7-x}$ Films Deposited by Using Various Carboxylate Solutions

In this work, four fluorine-free solutions based on various carboxylates (propionates, butyrates, valerates, and hexanoates, respectively) were prepared and used for deposition of YBCO films on LaAlO$_3$ single-crystal substrates, in order to further understand the role of precursors on properties of the final films. After the same pyrolysis and sintering processes, the films from propionates and butyrates show pure YBCO phase and were epitaxially grown, as determined by X-ray diffractometer analysis. There are clear differences in morphologies of these four films, i.e., the films from propionates and butyrates exhibit platelike grains without distinct grain boundaries, while almost randomly orientated grains were observed on the surface of the other two films. As a result, we noticed significant discrepancies on their superconducting performance. The films from propionates and butyrates give Jc values (at 77 K, self-field) of 2.1 MA/cm$^2$ and 1.3 MA/cm$^2$, respectively, while no superconducting transition above 70 K was observed in the other two films. A relatively larger amount of carbonaceous residue left as a by-product after decomposition of carboxylates with longer ligands, particularly under fast pyrolysis and sintering processes, could be one of the explanations of the poor superconductivity in the films from the valerate and hexanoate-based precursors.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Atomic scale modelling and materials, Universidad Autonoma de Barcelona
Authors: Yue, Z. (Intern), Torres, P. (Ekstern), Norby, P. (Intern), Wulff, A. C. (Intern), Grivel, J. (Intern)
Number of pages: 4
Pages: 6600204
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: IEEE Transactions on Applied Superconductivity
Volume: 25
Issue number: 3
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Complete relaxation of residual stresses during reduction of solid oxide fuel cells

To assess the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. This work reports further details on a newly discovered creep phenomenon, accelerated creep, taking place during the reduction of the anode. This relaxes stresses at a much higher rate ($\approx 10^4$) than creep during operation. The phenomenon has previously been studied by simultaneous loading and reduction. With the recorded high creep rates, the stresses at the time of reduction should reduce significantly over minutes. In this work the stresses are measured in-situ before and after the reduction by use of XRD. The phenomenon of accelerated creep has to be considered both in the production of stacks and in the analysis of the stress field in a stack based on anode supported SOFCs.

General information
Computational Analysis and Design of New Materials for Metal-Air Batteries

In the last decade, great effort has been paid to the development of next generation batteries. Metal-O2/Air batteries (Li-, Na-, Mg-, Al-, Fe- and Zn-O2 batteries) in both aqueous and nonaqueous (aprotic) electrolytes have gained much attention. Metal-air batteries have high theoretical specific gravimetric energy. In the case of Li-O2, it is comparable to that of gasoline. Thus, Li-O2 batteries could be attractive for electric vehicle manufacturers since the energy storage capacity accessible by commercially available Li-ion technology is too low to solve increasing capacity demands. However, current Li-O2 batteries suffer from several drawbacks, e.g. dendrite formation, poor rechargeability and low capacity caused by the so-called “sudden death” at its cathode during the discharge process due to insulating discharge products. This thesis is devoted to understand the charge transport in the main reaction products of emerging nonaqueous Li- and Na-O2 batteries at the atomistic level using the Density Functional Theory (DFT) method to address the latter problem. The role of cathode-electrolyte interface on charge transport and the implication of impurities from the air, particularly the effect of CO2 poisoning, in the performance of the battery are addressed. The present work involves computational investigations of different charge transport mechanisms, i.e. ionic, coherent electron, and polaronic transport. In order to validate the outcome from DFT calculations, results are compared with relevant experiments and show a notable agreement. The results of charge transport calculations in bulk Li2O2 (main discharge product in Li-O2 batteries) revealed that though it is a wide bandgap insulator (4.96 eV) it could offer fast ionic conduction with an activation barrier of 0.40 eV. Similarly, an accessible energy barrier for sodium ion diffusion is obtained in Na2O2 and in NaO2 (main discharge products in Na-O2 batteries). The transport mechanisms at the cathode-electrolyte interfaces, i.e. Li2O2@Li2CO3 interface, are also examined. Lithium vacancies accumulate at the peroxide side of this interface, reducing the coherent electron transport by two to three orders of magnitude compared to bulk pristine Li2O2. In contrast, the Li2O2@Li2CO3 interface shows an improved ionic conduction. For polaronic transport significant differences are also found in these two scenarios. In bulk Li2O2 the polaronic transport at room temperature is restricted to hole polarons, whereas electron polarons display very high hopping barriers (> 1.0 eV). By contrast, it is possible to have good mobilities for electron polarons at the Li2O2@Li2CO3 interface. Finally, our studies on the reaction mechanism of Li2O2 revealed that the CO2 poisoning, even at low concentrations of CO2 effectively blocks the step nucleation site and remarkably increases overpotentials and decreases the capacity of the battery.
Computationally Efficient Model of An Active Magnetocaloric Regenerator

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Authors: Tahavori, M. (Ekstern), Veje, C. (Ekstern), Lei, T. (Intern), Nielsen, K. K. (Intern), Engelbrecht, K. (Intern)
Number of pages: 5
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 5th IEEE International Conference on Control Systems, Computing and Engineering
Publisher: IEEE
Main Research Area: Technical/natural sciences
Source: FindIt
Source-ID: 2287342363
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Computational thermodynamics in electric current metallurgy
A priori derivation for the extra free energy caused by the passing electric current in metal is presented. The analytical expression and its discrete format in support of the numerical calculation of thermodynamics in electric current metallurgy have been developed. This enables the calculation of electric current distribution, current induced temperature distribution and free energy sequence of various phase transitions in multiphase materials. The work is particularly suitable for the study of magnetic materials that contain various magnetic phases. The latter has not been considered in literature. The method has been validated against the analytical solution of current distribution and experimental observation of microstructure evolution. It provides a basis for the design, prediction and implementation of the electric current metallurgy. The applicability of the theory is discussed in the derivations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, The Open University
Authors: Bhowmik, A. (Intern), Qin, R. (Ekstern)
Pages: 1560-1563
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science and Technology
Volume: 31
Issue number: 13a
ISSN (Print): 0267-0836
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.43 SJR 0.814 SNIP 0.812
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.632 SNIP 0.764 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.788 SNIP 1.005 CiteScore 1.1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.636 SNIP 0.868 CiteScore 0.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Computation of Effective Steady-State Creep of Porous Ni–YSZ Composites with Reconstructed Microstructures

This paper investigates the effective steady-state creep response of porous Ni–YSZ composites used in solid oxide fuel cell applications by numerical homogenization based on three-dimensional microstructural reconstructions and steadystate creep properties of the constituent phases. The Ni phase is found to carry insignificant stress in the composite and has a negligible role in the effective creep behavior. Thus, when determining effective creep, porous Ni–YSZ composites can be regarded as porous YSZ in which the Ni phase is counted as additional porosity. The stress exponents of porous YSZ are the same as that of dense YSZ, but the effective creep rate increases by a factor of 8–10 due to porosity. The relationship of creep rate and volume fraction of YSZ computed by numerical homogenization is underestimated by most existing analytical models. The Ramakrishnan–Arunchalam creep model provides the closest approximation among all analytical models.
Journal: American Ceramic Society. Journal
Volume: 98
Issue number: 9
ISSN (Print): 0002-7820
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1 SNIP 1.369
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.017 SNIP 1.42 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.192 SNIP 1.628 CiteScore 2.78
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.168 SNIP 1.481 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.277 SNIP 1.523 CiteScore 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.961 SNIP 1.465 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.455 SNIP 1.53
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.546 SNIP 1.433
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.444 SNIP 1.454
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.265 SNIP 1.439
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.126 SNIP 1.447
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.205 SNIP 1.635
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.56 SNIP 1.766
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.906 SNIP 1.805
Scopus rating (2002): SJR 2.109 SNIP 1.916
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.344 SNIP 2.399
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.2 SNIP 2.069
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.415 SNIP 2.528
Original language: English
Controlling the Activity and Stability of Pt-Based Electrocatalysts By Means of the Lanthanide Contraction

In order to reduce the Pt loading at the cathode of proton exchange membrane fuel cells (PEMFCs) more active and stable catalysts are needed to drive the oxygen reduction reaction. Most research has focussed on achieving this by alloying Pt with Fe, Co, Ni or Cu [1,2]. However, these compounds typically degrade under PEMFC conditions, due to dealloying. Alloys of Pt and lanthanides may be inherently less prone to dealloying under reactions conditions, due to their negative enthalpy of formation [2-4].

Herein we present a systematic study on the trends in activity of seven novel Pt-lanthanide electrodes (Pt5La, Pt5Ce, Pt5Sm, Pt5Gd, Pt5Tb, Pt5Dy and Pt5Tm). The materials are highly active, presenting a 3 to 6-fold activity enhancement over Pt [3-5], amongst the most active polycrystalline Pt-based catalyst ever reported. Moreover, our recent study showed that PtxGd is highly active in the nanoparticulate form [6]. On the bulk alloys, a Pt overlayer with a thickness of few Pt layers is formed onto the bulk alloys by acid leaching (Fig. 1A) [3-5]. The ORR activity versus the lattice parameter obtained by X-ray diffraction measurements follows a volcano relationship (Fig. 1B). Furthermore, we explain the trends in stability, and present the lattice parameter as a new descriptor that controls both the activity and stability of these materials. Using the lanthanide contraction we demonstrate that the electrocatalytic performance can be engineered by tuning the Pt-Pt distance.

CO₂ Fixation by Membrane Separated NaCl Electrolysis

Atmospheric concentrations of carbon dioxide (CO₂), a major cause of global warming, have been rising due to industrial development. Carbon capture and storage (CCS), which is regarded as the most effective way to reduce such atmospheric CO₂ concentrations, has several environmental and technical disadvantages. Carbon capture and utilization (CCU), which has been introduced to cover such disadvantages, makes it possible to capture CO₂, recycling byproducts as resources. However, CCU also requires large amounts of energy in order to induce reactions. Among existing CCU technologies, the process for converting CO₂ into CaCO₃ requires high temperature and high pressure as reaction conditions. This study proposes a method to fixate CaCO₃ stably by using relatively less energy than existing methods. After forming NaOH absorbent solution through electrolysis of NaCl in seawater, CaCO₃ was precipitated at room temperature and pressure. Following the experiment, the resulting product CaCO₃ was analyzed with Fourier transform infrared spectroscopy (FT-IR); field emission scanning electron microscopy (FE-SEM) image and X-ray diffraction (XRD) patterns were also analyzed. The results showed that the CaCO₃ crystal product was high-purity calcite. The study shows a successful method for fixating CO₂ by reducing carbon dioxide released into the atmosphere while forming high-purity CaCO₃.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

CO₂ Fixation by Membrane Separated NaCl Electrolysis

Atmospheric concentrations of carbon dioxide (CO₂), a major cause of global warming, have been rising due to industrial development. Carbon capture and storage (CCS), which is regarded as the most effective way to reduce such atmospheric CO₂ concentrations, has several environmental and technical disadvantages. Carbon capture and utilization (CCU), which has been introduced to cover such disadvantages, makes it possible to capture CO₂, recycling byproducts as resources. However, CCU also requires large amounts of energy in order to induce reactions. Among existing CCU technologies, the process for converting CO₂ into CaCO₃ requires high temperature and high pressure as reaction conditions. This study proposes a method to fixate CaCO₃ stably by using relatively less energy than existing methods. After forming NaOH absorbent solution through electrolysis of NaCl in seawater, CaCO₃ was precipitated at room temperature and pressure. Following the experiment, the resulting product CaCO₃ was analyzed with Fourier transform infrared spectroscopy (FT-IR); field emission scanning electron microscopy (FE-SEM) image and X-ray diffraction (XRD) patterns were also analyzed. The results showed that the CaCO₃ crystal product was high-purity calcite. The study shows a successful method for fixating CO₂ by reducing carbon dioxide released into the atmosphere while forming high-purity CaCO₃.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Yonsei University, Korea Institute of Geoscience and Mineral Resources
Authors: Park, H. S. (Ekstern), Lee, J. S. (Ekstern), Han, J. (Intern), Park, S. (Ekstern), Park, J. (Ekstern), Min, B. R. (Ekstern)
Number of pages: 12
Pages: 8704-8715
Publication date: 2015
Main Research Area: Technical/natural sciences
Creation of High Mobility Two-Dimensional Electron Gases via Strain Induced Polarization at an Otherwise Nonpolar Complex Oxide Interface

The discovery of two-dimensional electron gases (2DEGs) in SrTiO$_3$-based heterostructures provides new opportunities for nanoelectronics. Herein, we create a new type of oxide 2DEG by the epitaxial-strain-induced polarization at an otherwise nonpolar perovskite-type interface of CaZrO$_3$/SrTiO$_3$. Remarkably, this heterointerface is atomically sharp and exhibits a high electron mobility exceeding 60 000 cm$^2$ V$^{-1}$ s$^{-1}$ at low temperatures. The 2DEG carrier density exhibits a critical dependence on the film thickness, in good agreement with the polarization induced 2DEG scheme.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Center for Electron Nanoscopy, Imaging and Structural Analysis, Atomic scale modelling and materials, University of Copenhagen
Pages: 1849–1854
Publication date: 2015
Main Research Area: Technical/natural sciences
CsH₂PO₄/NdPO₄ Composites as Proton Conducting Electrolytes for Intermediate Temperature Fuel Cells

Composite proton conducting materials based on cesium dihydrogen phosphate and neodymium phosphate hydrate were prepared and investigated in terms of X-ray diffraction, thermogravimetry, conductivity, stability and fuel cell performance. At 150°C the conductivity was $1.8 \times 10^{-6}$ S cm$^{-1}$ for the pristine cesium dihydrogen phosphate and $0.8 \times 10^{-4}$ S cm$^{-1}$ for neodymium phosphate hydrate, while that of the composite containing 29 mol% neodymium phosphate and 71 mol% cesium dihydrogen phosphate was $0.4 \times 10^{-2}$ S cm$^{-1}$. It was proposed that the interaction between the two components establishes a dynamic hydrogen bonding network enabling efficient proton conduction long before the development of the
extensive phase disordering of the superprotonic transition. The presence of thermally stable hydrate water present in neodymium phosphate may also play a role in improving both conductivity and stability of the solid acid. The electromotive force, open circuit voltage and fuel cell performance were measured as demonstration of the material application.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Anfimova, T. (Intern), Jensen, A. H. (Intern), Christensen, E. (Intern), Jensen, J. O. (Intern), Bjerrum, N. J. (Intern), Li, Q. (Intern)
Pages: F436-F441
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochemical Society. Journal
Volume: 162
Issue number: 4
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.611 SNIP 1.54
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.519 SNIP 1.484
Degradation Studies on LiFePO$_4$ cathode

In this paper we examine a laboratory LiFePO$_4$ (LFP) cathode and propose a simple model that predicts the electrode capacity as function of C-rate, number of cycles and calendar time. Microcracks were found in Li$_{1-x}$FePO$_4$ particles in a degraded LFP electrode and low-acceleration voltage (1 kV) FIB/SEM analysis allowed us to obtain phase contrast between FePO$_4$ and LiFePO$_4$. The evolution of micro-cracks is expected to increase the concentration of LFP particles which are not electronically accessible and thus cause a loss in capacity.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Atomic scale modelling and materials, Department of Electrical Engineering
Authors: Scipioni, R. (Intern), Jørgensen, P. S. (Intern), Hjelm, J. (Intern), Norby, P. (Intern), Rasmussen, C. N. (Intern), Jensen, S. H. (Intern)
Pages: 97-106
Publication date: 2015
Conference: 226th Meeting of the Electrochemical Society (ECS) and 7th Meeting of the Mexico Section of the Electrochemical Society ECS and SMEQ Joint International Meeting, Cancun, Mexico, 05/10/2014 - 05/10/2014
Main Research Area: Technical/natural sciences

Publication information

Journal: ECS Transactions
Volume: 64
Issue number: 22
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
Depth profiling the solid electrolyte interphase on lithium titanate (Li4Ti5O12) using synchrotron-based photoelectron spectroscopy

The presence of a surface layer on lithium titanate (Li4Ti5O12, LTO) anodes, which has been a topic of debate in scientific literature, is here investigated with tunable high surface sensitive synchrotron-based photoelectron spectroscopy (PES) to obtain a reliable depth profile of the interphase. Li||LTO cells with electrolytes consisting of 1 M lithium hexafluorophosphate dissolved in ethylene carbonate:diethyl carbonate (LiPF6 in EC:DEC) were cycled in two different voltage windows of 1.0-2.0 V and 1.4-2.0 V. LTO electrodes were characterized after 5 and 100 cycles. Also the pristine electrode as such, and an electrode soaked in the electrolyte were analyzed by varying the photon energies enabling depth profiling of the outermost surface layer. The main components of the surface layer were found to be ethers, P-O containing compounds, and lithium fluoride.
Design and experimental tests of a rotary active magnetic regenerator prototype

A rotary active magnetic regenerator (AMR) prototype with efficiency and compact design as focus points has been designed and built. The main objective is to demonstrate improved efficiency for rotary devices by reducing heat leaks from the environment and parasitic mechanical work losses while optimizing the utilization of the magnetized volume. Heat transfer calculations combined with 1D AMR modeling have revealed the necessity for an insulating air gap between magnet and regenerator when designing for high efficiency. 2D finite difference AMR modeling capturing the interplay between heat transfer fluid flow and an inhomogenous time-varying magnetic field in the individual regenerator beds has been used in the design process. For one operating point a COP of 3.1 at a temperature span of 10.2 K and a cooling power of 103 W were measured. Major issues limiting the performance have been identified and improvements are outlined for future work. © 2015 Elsevier Ltd and IIR. All rights reserved.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Pages: 14-21
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: International Journal of Refrigeration
Volume: 58
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.309 SNIP 1.737
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.841 SNIP 1.646
Scopus rating (2006): SJR 1.5 SNIP 1.629
Scopus rating (2005): SJR 1.409 SNIP 1.718
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.193 SNIP 1.933
Scopus rating (2003): SJR 1.241 SNIP 1.542
Scopus rating (2002): SJR 1.592 SNIP 1.807
Scopus rating (2001): SJR 1.775 SNIP 1.86
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.001 SNIP 1.279
Scopus rating (1999): SJR 0.824 SNIP 1.213
Original language: English
Magnetic refrigeration, Design, Model, Efficiency, Experimental
DOIs:
10.1016/j.ijrefrig.2015.05.004
Publication: Research - peer-review › Journal article – Annual report year: 2015
Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery

Energy safety is a vital issue of the global future. Together with developing renewable and eco-friendly energy sources, recovering waste energy is no less of an important issue. It is estimated that 60% of energy converted in most of today’s energy processes nowadays is waste, mainly in the form of heat. Using thermoelectric generators, which convert heat into electricity, is a promising way to recover waste energy. However, the efficiency of thermal-to-electricity converters needs to be improved in order to be widely applied in practice. Despite the fact that significant amount of efforts have been focused on material development, realizing high efficient thermoelectric generators from such well-developed materials is still limited. Moreover, no single thermoelectric material could withstand the wide temperature range required to boost efficiency of TEGs. By segmentation of different TE materials which operate optimally in each temperature range, this study aims at developing high performance segmented TEGs for medium-high (450 – 850 K) temperature application. The research is focused on the challenges in joining and minimizing the contact resistances between different TE materials and with metal electrode.

One-dimensional numerical modeling was employed to design and predict the efficiency of segmented materials built up from most of today’s state-of-the-art thermoelectric materials. Combinations of materials that would deliver the highest conversion efficiency in different temperature ranges of 300 – 700, and 900 – 1100 K are considered. The obtained results reveals that segmented thermoelectric generator comprising of Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe/SiGe as p-leg and either segmented Bi2Te3/PbTe/SiGe or Bi2Te3/Ba0.08La0.05Yb0.04Co4Sb12/La3Te4 as n-leg working in 300 – 1100 K temperature range could achieve a maximum efficiency of 18.2 %. In lower working temperature ranges of 300 – 700 and 300 – 900 K, the maximum efficiencies are 13.5 and 16.6 %, respectively for segmented TEGs of p-leg Bi0.6Sb1.4Te3/TAGS ((AgSbTe)0.15(GeTe)0.85) with n-leg Bi2Te3/PbTe and p-leg Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe with n-leg Bi2Te3/PbTe/SiGe. The results could provide a guideline to develop high efficiency segmented thermoelectric generators. Based on these theoretical results, segmentation of half-Heusler alloys and Bi2Te3 materials was selected for further study.

Firstly, the joining between thermoelectric p- and n-type half-Heusler (HH) alloys and silver electrode at hot side was developed. A fast-hot pressing method was introduced to directly join the HH materials with silver interconnecting layer. The method was also compared with the conventional joining method where a third material is used as filler. Microstructures and interfacial chemical evolution at the joining interfaces were investigated using scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The transport properties of the joint, including thermopower across the interfaces and contact resistance as a function of temperature were studied. With fast hot pressing method, the contact resistance between HH alloys and Ag-electrode could be significantly reduced by about 50 %. Moreover, by avoiding a third filler material, the method limits the formation of new phases at contact interface which might degrade the overall thermoelectric properties. This work is a crucial step to make segmented HH/BiTe TEG.

Then, p- and n-type segmented legs of bismuth tellurides and half-Heusler alloys were built and characterized. Segmentation of bismuth tellurides to half-Heusler/Ag was processed at temperature 493 K, pressure 30 MPa in vacuum using Ag10Sn90 solder as filler. Interface microstructural evolution and thermoelectric properties of segmented legs were then investigated. The contact resistance of the join parts as a function of temperature was measured from room temperature to 473 K. Numerical modeling was used to evaluate the influence of measured contact resistances on the final power generating properties of the obtained segmented legs and their unicouple. Under working temperature from 323 to 873 K, the obtained p-segmented legs could deliver a power density of 0.3 Wcm-2 and maximum voltage of 115 mV. With the same condition, the power density and maximum voltage generated by n-segmented leg were 0.25 Wcm-2 and 102 mV. These values are significantly smaller than calculation data. The reason is possibly due to the contact between BiTe and electrode at the cold end, thus improvement of the cold side contact was made. At temperature gradient of 498 K, the maximum power density of the improved n-segmented leg was 0.8 Wcm-2, giving a maximum efficiency of 4.5%.

General information

State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage
Authors: Pham, H. N. (Intern), Pryds, N. (Intern), Van Nong, N. (Intern), Linderoth, S. (Intern)
Number of pages: 124
Publication date: 2015

Publication information

Place of publication: Roskilde
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
ry.pdf
Publication: Research › Ph.D. thesis – Annual report year: 2015
Design of two-photon molecular tandem architectures for solar cells by ab initio theory
An extensive database of spectroscopic properties of molecules from ab initio calculations is used to design molecular complexes for use in tandem solar cells that convert two photons into a single electron–hole pair, thereby increasing the output voltage while covering a wider spectral range. Three different architectures are considered: the first two involve a complex consisting of two dye molecules with appropriately matched frontier orbitals, connected by a molecular diode. Optimized combinations of dye molecules are determined by taking advantage of our computational database of the structural and energetic properties of several thousand porphyrin dyes. The third design is a molecular analogy of the intermediate band solar cell, and involves a single dye molecule with strong intersystem crossing to ensure a long lifetime of the intermediate state. Based on the calculated energy levels and molecular orbitals, energy diagrams are presented for the individual steps in the operation of such tandem solar cells. We find that theoretical open circuit voltages of up to 1.8 V can be achieved using these tandem designs. Questions about the practical implementation of prototypical devices, such as the synthesis of the tandem molecules and potential loss mechanisms, are addressed.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad Autónoma de Madrid, Max Planck Institute for the Structure and Dynamics of Matter
Authors: Ørnsø, K. B. (Intern), García Lastra, J. M. (Intern), De La Torre, G. (Ekstern), Rubio, A. (Ekstern), Thygesen, K. S. (Intern)
Pages: 3018-3025
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication Information
Journal: Chemical Science
Volume: 6
ISSN (Print): 2041-6520
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.44 SJR 4.475 SNIP 1.67
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.74 SNIP 1.749 CiteScore 9.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 4.991 SNIP 1.745 CiteScore 8.99
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 4.675 SNIP 1.587 CiteScore 8.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.146 SNIP 1.819 CiteScore 8.18
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 4.33 SNIP 1.799 CiteScore 7.01
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Original language: English
Electronic versions:
Tandem.pdf
DOIs:
10.1039/C4SC03835E

Bibliographical note
© The Royal Society of Chemistry 2015
Source: PublicationPreSubmission
Source-ID: 108096216
Publication: Research - peer-review → Journal article – Annual report year: 2015
Development and Manufacture of Polymer-based Electrochromic Devices

The field of organic electrochromics is reviewed here, with particular focus on how the "electrochromic" as a functional material can be brought from the current level of accurate laboratory synthesis and characterization to the device and application level through a number of suited roll-to-roll methods compatible with upscaling and manufacture. The successful approaches to operational devices are presented in detail, as well as areas where future research would have a high impact and accelerate the development such as highly conducting and transparent substrates, electrolytes adapted for multilayer application and morphologically stable conjugated polymers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Clayton State University
Authors: Jensen, J. (Intern), Hösel, M. (Intern), Dyer, A. L. (Ekstern), Krebs, F. C. (Intern)
Pages: 2073–2090
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 25
Issue number: 14
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Original language: English
DOIs:
10.1002/adfm.201403765
Source: PublicationPreSubmission
Source-ID: 106310650
Publication: Research - peer-review › Journal article – Annual report year: 2015
Development of high temperature PEM fuel cells. Simplification and CO tolerance mapping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Fernandez, S. M. (Intern), Vassiliev, A. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 27
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
Side event to European Fuel Cell - Piero Lunghi Conference & Exhibition
Source: PublicationPreSubmission
Source-ID: 127806915
Publication: Research › Sound/Visual production (digital) – Annual report year: 2016

Development of Lab-to-Fab Production Equipment Across Several Length Scales for Printed Energy Technologies, Including Solar Cells

We describe and review how the scaling of printed energy technologies not only requires scaling of the input materials but also the machinery used in the processes. The general consensus that ultrafast processing of technologies with large energy capacity can only be realized using roll-to-roll methods is taken as a premise, and thus the progression from a highly successful laboratory technique (i.e., spin coating) to large-scale roll-to-roll equipment is described in terms of all of the intermediate steps that must be available to make the transfer possible. Spin coating is compatible with materials availability on the small scale and efficient scaling of equipment is a demanding task that must be performed in parallel with increasing materials availability. We outline that 3–5 processing platforms are necessary to efficiently take the laboratory technology to a version that represents the lower end of the industrial scale. The machinery bridges the gap through firstly achieving improved ink efficiency without surface contact, followed by better ink efficiency at higher speeds, and finally large-area processing at high speed with very high ink efficiency.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Hösel, M. (Intern), Dam, H. F. (Intern), Krebs, F. C. (Intern)
Pages: 293–304
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Technology
Volume: 3
Issue number: 4
ISSN (Print): 2194-4288
Ratings:
Web of Science (2017): Indexed yes
Scopus rating (2016): SJR 0.283 SNIP 0.13 CiteScore 0.66
Scopus rating (2015): SNIP 0.103 SJR 0.163 CiteScore 0.21
Web of Science (2015): Indexed yes
Scopus rating (2014): SNIP 0.564 SJR 1.681
Web of Science (2014): Indexed yes
ISI indexed (2013): ISI indexed no
Original language: English
Organic photovoltaics, Perovskites, Polymers, Roll-to-roll processing, Solar cells
Electronic versions:
Development_of_Lab_to_Fab.pdf
DOIs:
10.1002/ente.201402140
Dictionary Based Segmentation in Volumes

We present a method for supervised volumetric segmentation based on a dictionary of small cubes composed of pairs of intensity and label cubes. Intensity cubes are small image volumes where each voxel contains an image intensity. Label cubes are volumes with voxelwise probabilities for a given label. The segmentation process is done by matching a cube from the volume, of the same size as the dictionary intensity cubes, to the most similar intensity dictionary cube, and from the associated label cube we get voxel-wise label probabilities. Probabilities from overlapping cubes are averaged and hereby we obtain a robust label probability encoding. The dictionary is computed from labeled volumetric image data based on weighted clustering. We experimentally demonstrate our method using two data sets from material science – a phantom data set of a solid oxide fuel cell simulation for detecting three phases and their interfaces, and a tomogram of a glass fiber composite used in wind turbine blades for detecting individual glass fibers.

General Information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, Department of Wind Energy, Composites and Materials Mechanics, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Number of pages: 12
Pages: 504-515
Publication date: 2015

Host publication information
Title of host publication: Image Analysis : 19th Scandinavian Conference, SCIA 2015 Copenhagen, Denmark, June 15-17, 2015 Proceedings
Publisher: Springer Science+Business Media B.V.
ISBN (Print): 978-3-319-19664-0
ISBN (Electronic): 978-3-319-19665-7
Series: Lecture Notes in Computer Science
ISSN: 0302-9743
BFI conference series: Scandinavian Conference on Image Analysis (5010789)
Main Research Area: Technical/natural sciences
Conference: 19th Scandinavian Conference on Image Analysis, Copenhagen, Denmark, 15/06/2015 - 15/06/2015
Volume segmentation, Materials images, X-ray tomography, Learning dictionaries, Glass fiber segmentation
Electronic versions:
DOIs:
10.1007/978-3-319-19665-7_43

Relations
Projects:
Dictionary Based Segmentation in Volumes
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Dictionary Based Segmentation in Volumes
Method for supervised segmentation of volumetric data. The method is trained from manual annotations, and these annotations make the method very flexible, which we demonstrate in our experiments. Our method infers label information locally by matching the pattern in a neighborhood around a voxel to a dictionary, and hereby accounts for the volume texture.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, Department of Wind Energy, Composites and Materials Mechanics, Department of Energy Conversion and Storage,
Direct Coal Oxidation In Modified Solid Oxide Fuel Cells

Hybrid direct carbon fuel cells employ a classical solid oxide fuel cell together with carbon dispersed in a carbonate melt on the anode side. In a European project, the utilization of various coals has been investigated with and without addition of an oxidation catalyst to the carbon-carbonate slurry or anode layer. The nature of the coal affects both open circuit voltage and power output. Highest OCV and power densities were observed for bituminous coal and by adding manganese oxide or praseodymium-doped ceria to the carbon/carbonate mixture. Comparing the carbon black fueled performance of an anode supported (315 µm anodes) and cathode supported cell (15 µm anode) indicates a superior performance of the former. Using un-catalyzed biomass (charcoal) as fuel results in an OCV of 941 mV and a maximum power density of 78 mW/cm² at 755ºC similar to the power output of manganese oxide catalyzed bituminous coal (73 mW/cm²).

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General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Centro Nacional del Hidrogeno
Authors: Deleebeeck, L. (Intern), Gil, V. (Intern), Ippolito, D. (Intern), Campana, R. (Ekstern), Kammer Hansen, K. (Intern), Holtappels, P. (Intern)
Pages: 2685-2694
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 68
Issue number: 1
ISSN (Print): 1938-5862

Ratings:

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<td>SJR 0.262, SNIP 0.284, CiteScore 0.36</td>
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ISI indexed (2013): ISI indexed no
Direct measurements of the magnetic entropy change

An experimental device that can accurately measure the magnetic entropy change, $\Delta s$, as a function of temperature, $T$, and magnetic field, $H$, is presented. The magnetic field source is in this case a set of counter-rotating concentric Halbach-type magnets, which produce a highly homogeneous applied field with constant orientation. The field may be varied from 0 to 1.5 T in a continuous way. The temperature stability of the system is controlled to within $\pm 10$ mK and the standard range for the current setup is from 230 K to 330 K. The device is under high vacuum and we show that thermal losses to the ambient are negligible in terms of the calorimetric determination of the magnetic entropy change, while the losses cannot be ignored when correcting for the actual sample temperature. We apply the device to two different types of samples; one is commercial grade Gd, i.e., a pure second-order phase transition material, while the other is Gd$_{5}$Si$_{2}$Ge$_{2}$, a first order magnetic phase transition material. We demonstrate the device’s ability to fully capture the thermal hysteresis of the latter sample by following appropriate thermal resetting scheme and magnetic resetting scheme. © 2015 AIP Publishing LLC.
Dispenser printed thermoelectric generators

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Fraunhofer Institut für Werkstoff- und Strahltechnik, Dresden University of Technology
Authors: Stepień, L. (Ekstern), Roch, A. (Ekstern), Schlaier, S. (Ekstern), Abt, M. (Ekstern), Hoch, C. (Ekstern), Dani, I. (Ekstern), Van Nong, N. (Intern), Lukowicz, M. V. (Ekstern), Leyens, C. (Ekstern)
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 9C.2
Main Research Area: Technical/natural sciences
Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors
Authors: Fenini, F. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-26
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E26_DTU_Sustain_2015.pdf

Bibliographical note
Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Dynamic behavior of impurities and native components in model LSM microelectrodes on YSZ

Strontium-doped lanthanum manganese is a widely used cathode material in solid oxide fuel cells. Segregation phenomena can have a critical impact on performance and durability, especially when they cause active interfaces to degrade. The segregation behavior in polarized and non-polarized strontium-doped lanthanum manganese \((\text{La}_{0.75}\text{Sr}_{0.25})_{0.95}\text{MnO}_3\) microelectrodes with a diameter of 100 μm and a thickness of ~500 nm on an yttria-stabilized zirconia electrolyte were analyzed post-mortem after ~200 h at temperatures up to 850 °C. Time-of-flight secondary ion mass spectrometry was used to study the dynamic behavior of the native components (La, Sr, Mn) and selected impurities (Si, K, Na) both laterally and in-depth. Manganese was found to be especially mobile and showed both segregation onto the electrolyte as a result of temperature and polarization and dissolution into the electrolyte below the microelectrodes. All native components showed a complex in-depth dynamic behavior, and a nanoscale in-depth analysis of the electrode-electrolyte interface revealed the formation of a well-defined lanthanum zirconate layer. The selected impurities segregated to the electrolyte and microelectrode surfaces and Na- and K-rich layers formed at different depths.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry
Authors: Norrman, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern)
Number of pages: 15
Pages: 87679-87693
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: R S C Advances
Volume: 5
Issue number: 106
ISSN (Print): 2046-2069
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Dynamic rotor mode in antiferromagnetic nanoparticles

We present experimental, numerical, and theoretical evidence for an unusual mode of antiferromagnetic dynamics in nanoparticles. Elastic neutron scattering experiments on 8-nm particles of hematite display a loss of diffraction intensity with temperature, the intensity vanishing around 150 K. However, the signal from inelastic neutron scattering remains above that temperature, indicating a magnetic system in constant motion. In addition, the precession frequency of the inelastic magnetic signal shows an increase above 100 K. Numerical Langevin simulations of spin dynamics reproduce all measured neutron data and reveal that thermally activated spin canting gives rise to an unusual type of coherent magnetic precession mode. This "rotor" mode can be seen as a high-temperature version of superparamagnetism and is driven by exchange interactions between the two magnetic sublattices. The frequency of the rotor mode behaves in fair agreement with a simple analytical model, based on a high-temperature approximation of the generally accepted Hamiltonian of the system. The extracted model parameters, such as the magnetic interaction and the axial anisotropy, are in excellent agreement with results from Mossbauer spectroscopy.
Ecodesign of organic photovoltaic modules from Danish and Chinese perspectives

The life cycle of a solar park made using organic photovoltaic (OPV) technology is assessed here. The modules have been fabricated in a pilot scale plant and they have been installed together with other components to evaluate the balance of system, in a solar park located in Denmark. Three possible waste management practices have been contemplated for the end of life of the solar park: recycling, incineration or the average local mix. The assessment of the environmental impacts of such a system reveals that silver used in the electrodes is overall the largest source of impacts, such as chemical pollution and metal depletion. The establishment of resource recovery systems for the end-of-life management of the OPV modules is therefore crucial to reduce overall environmental impacts. Liability on the manufacturers or on the operators should be implemented. The electricity produced from OPV solar parks yields similar footprints to other traditional energy technologies; e.g. coal and natural gas. However, when the efficiency of the OPV modules is increased from 1% to 5% they are comparable to other mature PV technologies already on the market. The effects of outsourcing or exporting the production of the OPV modules from Denmark to China have additionally been studied to determine the most advantageous configuration. The stakeholders should aim at anchoring the manufacturing of solar parks in countries with stringent emission standards and/or high technology efficiencies, e.g. Denmark, and at deploying them in countries with high solar radiation to maximise the environmental benefits of the PV technology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Espinosa Martinez, N. (Intern), Laurent, A. (Intern), Krebs, F. C. (Intern)
Pages: 2537-2550
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 8
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 10.027 SNIP 4.275 CiteScore 23.85
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.792 SNIP 4.034 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.02 SNIP 3.011 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.86 SNIP 2.594 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.743 SNIP 2.513 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.861 SNIP 2.41
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.045 SNIP 1.139
Economic Potential of Biomass from Unused Agriculture Land for Energy Use: Case of Croatia

In this paper the energy potential of biomass from growing short rotation coppice (SRC) on unused agricultural land in the Republic of Croatia was examined. At present, SRC is not completely recognized in Croatian legislative and considerations in energy strategy and action plans. The paper aspires to contribute to better understanding of the role SRC can take in national and local energy planning. The methodology is provided for regional analysis of biomass energy potential on unused agricultural land and for assessing the cost of the biomass at the power plant (PP) location considering transport distance, transport costs and size of the power plants up to 15 MWe, which was applied on the case of Croatian counties. Case studies have been analysed for optimal locations of such power plants depending on energy potential of SRC in various counties. Operation costs are also calculated for such power plants and appropriate size of seasonal heat storage is discussed for each case study. Case studies have shown the potential for use of previously unused agricultural land to help achieve national targets for renewable energy sources as well as reducing carbon dioxide emissions, help diversify the landscape and increase biodiversity. Through scenario approach, technical and energy potential of SRC is investigated and noticeable potential in Karlovac and Sisak-Moslavina Counties, due to large area of unused agricultural land in those counties. Energy potential of those counties is 2.2 PJ/year for Karlovac and 1.7 PJ/year for Sisak-Moslavina Country. With price of biomass at gate of power plant in best scenario reaching 44.7 €/t, novel systems of combined cooling, heating and power generation (CCHP) are not yet feasible, but SRC could be considered in already established central district heating systems.

General information
State: Published
Authors: Pfeifer, A. (Ekstern), Dominkovic, D. F. (Intern), Ćosić, B. (Ekstern)
Pages: 351-351
Publication date: 2015

Effectiveness of electronic stability control on single-vehicle accidents

Objective: This study aims at evaluating the effectiveness of electronic stability control (ESC) on single-vehicle injury accidents while controlling for a number of confounders influencing the accident risk. Methods: Using police-registered injury accidents from 2004 to 2011 in Denmark with cars manufactured in the period 1998 to 2011 and the principle of induced exposure, 2 measures of the effectiveness of ESC were calculated: The crude odds ratio and the adjusted odds ratio, the latter by means of logistic regression. The logistic regression controlled for a number of confounding factors, of which the following were significant. For the driver: Age, gender, driving experience, valid driving license, and seat belt use. For the vehicle: Year of registration, weight, and ESC. For the accident surroundings: Visibility, light, and location. Finally, for the road: Speed limit, surface, and section characteristics. Results: The present study calculated the crude odds ratio for ESC-equipped cars of getting in a single-vehicle injury accident as 0.40 (95% confidence interval [CI], 0.34-0.47) and the adjusted odds ratio as 0.69 (95% CI, 0.54-0.88). No difference was found in the effectiveness of ESC across the injury severity categories (slight, severe, and fatal). Conclusions: In line with previous results, this study concludes that ESC reduces the risk for single-vehicle injury accidents by 31% when controlling for various confounding factors related to the driver, the car, and the accident surroundings. Furthermore, it is concluded that it is important to control for human factors (at a minimum age and gender) in analyses where evaluations of this type are performed.

General information
State: Published
Organisations: Department of Transport, Traffic modelling and planning, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Lyckegaard, A. (Intern), Hels, T. (Intern), Bernhoft, I. M. (Intern)
Pages: 380-386
Effect of Aging on the Electrochemical Performance of LSM-YSZ Cathodes

Investigations of degradation mechanisms of solid oxide fuel cells are crucial for achieving a widespread commercialization of the technology. In this work, electrochemical impedance spectroscopy (EIS) was applied for studying the aging effect on LSM-YSZ cathodes exposed to humidified air at 900°C for up to 3000 h. EIS spectra were fitted by a transmission line model for estimating relevant parameters associated with the LSM/YSZ charge transfer reaction and the oxide ion conduction through the YSZ network. For the reference non-aged sample, the ionic conductivity values are the expected ones for YSZ with 1 eV activation energy and no dependency on oxygen partial pressure (pO2), while the charge transfer resistance presents an activation energy of 1.6 eV and is proportional to (pO2)−0.31±0.08. These values
agree with those reported in literature, validating the used model. The charge transfer resistance shows no clear tendency with aging time, while the ionic conductivity decreases up to ~79%. Accordingly, the electrochemically active thickness contracts from 60–135 μm to 45–60 μm. The changes observed in the cathode transport and electrochemical properties are mostly explained by the evolution of the phases present in agreement with results previously reported in the literature.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Consejo Nacional de Investigaciones Científicas y Tecnológicas, Meneta Advanced Shims Technology A/S
Authors: Baqué, L. C. (Ekstern), Jørgensen, P. S. (Intern), Zhang, W. (Intern), Hansen, K. V. (Intern), Søgaard, M. (Ekstern)
Pages: F971-F981
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Electrochemical Society
Volume: 162
Issue number: 9
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.608 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.611 SNIP 1.54
Effect of BaZrO₃/Ag hybrid doping to the microstructure and performance of fluorine-free MOD method derived YBa₂Cu₃O₇₋ₓ superconducting thin films

It is known that BaZrO₃ and Ag can improve the magnetic and transport performance of YBCO thin film through totally disparate ways. BaZrO₃ plays the role of flux pinning centers and Ag improves the transparency of the YBCO grain boundaries. However, similar research is rare on the fluorine-free derived YBCO films. In this research, BaZrO₃-doped, Ag-doped and BaZrO₃/Ag hybrid-doped YBCO films were synthesized through a fluorine-free metal–organic deposition method. BaZrO₃ was found to deteriorate the microstructure and performance of YBCO, while Ag-doping was found to enhance the crystallization of YBCO and resulted in a high Jc of 3.87 MA/cm² in self-field at 77 K. However, the microstructure and performance of the BaZrO₃/Ag hybrid-doped YBCO film showed that the positive impact of Ag-doping was totally overwhelmed by that of BaZrO₃.
Effect of chemical redox on Gd-doped ceria mass diffusion

The valence and size of cations influence mass diffusion and oxygen defects in ceria. Here we show that reduction of Ce\textsuperscript{4+} to Ce\textsuperscript{3+}, at high temperatures and low oxygen activity, activates fast diffusion mechanisms which depend on the aliovalent cation concentration. As a result, polycrystalline solid solutions with enhanced electrochemical properties are formed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Universidade Federal do ABC
Number of pages: 4
Pages: 18835-18838
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 37
ISSN (Print): 2050-7488
Effect of Co3O4 and Co3O4/CeO2 infiltration on the catalytic and electro-catalytic activity of LSM15/CGO10 porous cells stacks for oxidation of propene

The objective of this work was to study the effect of Co3O4 and Co3O4/CeO2 infiltration on the propene oxidation catalytic activity of a La0.85Sr0.15MnO3/Ce0.9Gd0.1O1.95 electrochemical porous cell stack (11 layers, 5 single cells in series). The effect of the infiltration of Co3O4 and Co3O4/CeO2 on the electrochemical properties of the porous cell stack was also investigated by electrochemical impedance spectroscopy (EIS). Co3O4 and Co3O4/CeO2 exhibited high catalytic activity for propene oxidation. The increase of propene oxidation rate with +4 V (0.8 V/cell) polarization reached 10% for the Co3O4 infiltrated reactor and 48% of efficiency at 300 °C. The Co3O4/CeO2 co-infiltration decreased the reactor polarization resistance, while Co3O4 infiltration had negligible effect on reactor electrochemical performance. The beneficial effect of CeO2 on the electrode activity was attributed to the increased concentration of stable oxygen species on the electrode surface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Ippolito, D. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 6
Pages: 23-28
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 159
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Effect of Sb Segregation on Conductance and Catalytic Activity at Pt/Sb-Doped SnO₂ Interface: A Synergetic Computational and Experimental Study

Antimony doped tin dioxide (ATO) is considered a promising support material for Pt-based fuel cell cathodes, displaying enhanced stability over carbon-based supports. In this work, the effect of Sb segregation on the conductance and catalytic activity at Pt/ATO interface was investigated through a combined computational and experimental study. It was found that Sb-dopant atoms prefer to segregate toward the ATO/Pt interface. The deposited Pt catalysts, interestingly, not only promote Sb segregation, but also suppress the occurrence of Sb³⁺ species, a charge carrier neutralizer at the interface. The conductivity of ATO was found to increase, to a magnitude close to that of activated carbon, with an increment of Sb concentration before reaching a saturation point around 10%, and then decrease, indicating that Sb enrichment at the
ATO surface may not always favor an increment of the electric current. In addition, the calculation results show that the presence of Sb dopants in ATO has little effect on the catalytic activity of deposited three-layer Pt toward the oxygen reduction reaction, although subsequent alloying of Pt and Sb could lower the corresponding catalytic activity. These findings help to support future applications of ATO/Pt-based materials as possible cathodes for PEMFC applications with enhanced durability under practical applications.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Atomic scale modelling and materials, SINTEF, QuantumWise A/S, Norwegian University of Science and Technology
Pages: 27782–27795
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: A C S Applied Materials and Interfaces
Volume: 7
Issue number: 50
ISSN (Print): 1944-8244
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 1.571 SNIP 0.931
- Web of Science (2010): Indexed yes
- Web of Science (2009): Indexed yes
- Original language: English
- Interface, Segregation, Electronic Transport, Catalyst, Fuel Cell
- DOIs: 10.1021/acsami.5b08966

**Publication: Research - peer-review › Journal article – Annual report year: 2015**

**Effect of stress on NiO reduction in solid oxide fuel cells: A new application of energy-resolved neutron imaging**

Recently, two new phenomena linking stress field and reduction rates in anode-supported solid oxide fuel cells (SOFCs) have been demonstrated, so-called accelerated creep during reduction and reduction rate enhancement and nucleation due to stress (Frandsen et al., 2014). These complex phenomena are difficult to study and it is demonstrated here that energy-resolved neutron imaging is a feasible technique for combined mechanics-chemical composition studies of SOFC
components, including commercially produced ones. Cermet anode supports, which prior to the measurements were reduced under varying conditions such as different temperatures, various times and different values of applied stress, have been measured. Thus, samples with different contents (and gradients) of Ni and NiO phases were investigated. The first Bragg edge transmission neutron measurements applied for the studies of the reduction progress in these samples were performed at two neutron beamline facilities (ISIS in the UK, Helmholtz Zentrum Berlin in Germany). The obtained results demonstrate the possibility to image and distinguish NiO and Ni phases within SOFC anode supports by energy-resolved neutron imaging and the potential of the neutron imaging method for in situ studies of reduction processes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Rutherford Appleton Laboratory, European Spallation Source ESS AB, Helmholtz–Zentrum Berlin für Materialien und Energie, Xnovo Technology ApS, University of California at Berkeley
Authors: Makowska, M. (Intern), Strobl, M. (Ekstern), Lauridsen, E. M. (Ekstern), Frandsen, H. L. (Intern), Tremsin, A. S. (Ekstern), Kardjilov, N. (Ekstern), Manke, I. (Ekstern), Kelleher, J. F. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 8
Pages: 401-408
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 48
ISSN (Print): 0021-8898
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.6 SNIP 2.078
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.235 SNIP 2.117
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.126 SNIP 2.101
Web of Science (2008): Indexed yes
Effect of surface shear on cube texture formation in heavy cold-rolled Cu-45 at%Ni alloy substrates

Two types of Cu-45 at%Ni alloy thin tapes with and without surface shear were obtained by different heavy cold rolling processes. The deformation and recrystallization textures of the two tapes were thoroughly investigated by electron back scattering diffraction technique. The results showed that a shear texture mainly covered the surface of the heavy deformed tapes because of the fraction between the surface of rolling mills and the thin tapes when the rolling force strongly reduced at high strain, which significantly reduced the fraction of rolling texture on the surface of the Cu-45at %Ni alloy thin tapes, retarded the cube grain growth during recrystallization and affected the strong cube texture formation after high temperature annealing.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Beijing University of Technology
Authors: Tian, H. (Intern), Suo, H. (Ekstern), Liang, Y. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern)
Number of pages: 5
Pages: 83-87
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 141
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.757 SNIP 0.935
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.792 SNIP 1.021 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 1.315 CiteScore 2.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.83 SNIP 1.237 CiteScore 2.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.924 SNIP 1.404 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.017 SNIP 1.568 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.059 SNIP 1.29
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.043 SNIP 1.276
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.979 SNIP 1.3
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.943 SNIP 1.31
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.846 SNIP 1.16
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.775 SNIP 1.167
Scopus rating (2004): SJR 0.644 SNIP 1.031
Scopus rating (2003): SJR 0.602 SNIP 0.828
Scopus rating (2002): SJR 0.594 SNIP 0.917
Scopus rating (2001): SJR 0.516 SNIP 0.767
Scopus rating (2000): SJR 0.438 SNIP 0.745
Scopus rating (1999): SJR 0.502 SNIP 0.632
Original language: English
Metals and alloys, Microstructure, Recrystallization, Texture, Alloys, Backscattering, Crystal microstructure, Crystallization, Geometry, Grain growth, Metal cladding, Metallurgy, Nickel, Recrystallization (metallurgy), Rolling, Shear flow, Textures, After high temperature, Cold rolling process, Electron back scattering diffraction techniques, Ni-alloy substrates, Recrystallization texture, Rolling texture, Shear texture, Cold rolling
DOIs:
10.1016/j.matlet.2014.09.046
Source: FindIt
Source-ID: 271117348
Publication: Research - peer-review › Journal article – Annual report year: 2015

Effect of Temperature Step Size on Calculating the Magnetic Entropy Change

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Authors: Neves Bez, H. (Intern), Insinga, A. R. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. R. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Effect_of_Temperature_Step.pdf
**Effects of constant voltage and constant current stress in PCBM:P3HT solar cells**

The aim of this work is the investigation of forward and reverse bias stress effects, cell self-heating and annealing in roll coated organic solar cells with PCBM:P3HT active layer. In reverse bias stress cells show a constant degradation over time. In forward current stress cells alternate degradation and annealing phases, which are explained through the high power dissipation during the current stress, and the consequent self-heating. The high temperature is able to recover the cell performances at least until a critical temperature is reached. The degradation can be explained by the following mechanisms: the decrease of the net generation rate (due to formation of exciton quenching centres or the reduction of exciton separation rate); the formation of small leaky paths between anode and cathode, which reduces the total current extracted from the cell. The stress-induced damage can be recovered by thermal annealing at 120 °C. © 2015 Elsevier Ltd. All rights reserved.
Effects of the fabrication process on the grain-boundary resistance in BaZr$_{0.9}$Y$_{0.1}$O$_{3-\delta}$

Correction for "Effects of the fabrication process on the grain-boundary resistance in BaZr0.9Y0.1O$_{3-\delta}$" by S. Ricote et al., J. Mater. Chem. A, 2014, 2, 16107–16115.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Colorado Fuel Cell Center, CoorsTek, Inc.
Authors: Ricote, S. (Ekstern), Bonanos, N. (Intern), Manerbino, A. (Ekstern), Sullivana, N. P. (Ekstern), Coorsc, W. G. (Ekstern)
Number of pages: 1
Pages: 12558
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 23
ISSN (Print): 2050-7488
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- ISI indexed (2013): ISI indexed no
- Web of Science (2013): Indexed yes
Original language: English
Electronic versions:
c5ta90117k.pdf
DOIs:
10.1039/c5ta90117k

Bibliographical note
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Source: FindIt
Effects of Yttrium and Iron co-doping on the high temperature thermoelectric properties of Ca$_3$Co$_4$O$_{9+δ}$

A series of Y and Fe co-doped Ca$_{3-x}$Y$_x$Co$_{4-y}$Fe$_y$O$_{9+δ}$ (0 ≤ x ≤ 0.3, 0 ≤ y ≤ 0.1) samples synthesized by auto-combustion reaction and followed by a spark plasma sintering (SPS) processing with the effects of Fe and Y doping on the high temperature (RT to 800 °C) thermoelectric properties were systematically investigated. For the Fe-doped system (x = 0, y = 0.1), the electrical resistivity (ρ) decreased over the whole measured temperature range, while the Seebeck coefficient (S) remained almost the same. For the co-doped system, at any fixed Fe doping content, both ρ and S tended to increase with increasing Y dopants; however, the effect is more substantial on ρ than on S, particularly in the low temperature regime. In contrast to ρ and S, the in-plane thermal conductivity (κ) is only slightly influenced by Y and Fe substitutions. Among all the investigated samples, the co-doped sample with x = 0.1 and y = 0.03 showed a decrease of ρ, enhanced power factor over the measured temperature range, and improved ZT at 800 °C as compared to un-doped Ca$_3$Co$_4$O$_{9+δ}$. 

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Wu, N. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern), Linderoth, S. (Intern)
Pages: 127–132
Publication date: 2015
Main Research Area: Technical/natural sciences
Elastocaloric cooling device: Materials and modeling
In the last decade we have witnessed the development of alternative solid-state cooling technologies based on so-called ferroic (caloric) effects. A large effort nowadays is devoted to investigating solid-state refrigeration using the magnetocaloric effect (change of temperature upon application of a magnetic field). However, the possibility of inducing a thermodynamic transition by means of mechanical stress (martensitic transformation), i.e. the elastocaloric effect in superelastic materials, opens up new routes for solid-state refrigeration. In the recent years a large elastocaloric effect was demonstrated in Ni-Ti-based, Cu-based as well as Fe-based shape memory alloys. Although these studies showed a great potential of the elastocaloric effect, there has not yet been much activities on development of elastocaloric cooling devices. Some ideas on elastocaloric cooling device have already been presented, but there is still a lack of knowledge and information about its actual cooling potential.

Elastocaloric effect of Ni-Ti wire for application in a cooling device
We report on the elastocaloric effect of a superelastic Ni-Ti wire to be used in a cooling device. Initially, each evaluated wire was subjected to 400 loading/unloading training cycles in order to stabilize its superelastic behavior. The wires were trained at different temperatures, which lead to different stabilized superelastic behaviors. The stabilized (trained) wires were further tested isothermally (at low strain-rate) and adiabatically (at high strain-rate) at different temperatures (from 312 K to 342 K). We studied the impact of the training temperature and resulting superelastic behavior on the adiabatic temperature changes. The largest measured adiabatic temperature change during loading was 25 K with a corresponding
21K change during unloading (at 322 K). A special focus was put on the irreversibilities in the adiabatic temperature changes between loading and unloading. It was shown that there are two sources of the temperature irreversibilities: the hysteresis (and related entropy generation) and the temporary residual strain immediately after unloading, respectively. The latter results in the temporary bending of the wire and reduced negative adiabatic temperature change. The paper also shows the impact of the applied strain on the adiabatic temperature changes as well as the distribution of the elastocaloric effect over the wire during loading in the case of two wires trained at different temperatures and the virgin wire, respectively. In the end, we propose guidelines about the required material properties for an efficient elastocaloric cooling device. © 2015 AIP Publishing LLC.
Electrical characterization of fluorinated benzothiadiazole based conjugated copolymer – a promising material for high-performance solar cells

Measurements of electrical conductivity, electron work function, carrier mobility of holes and the diffusion length of excitons were performed on samples of conjugated polymers relevant to polymer solar cells. A state of the art fluorinated benzothiadiazole based conjugated copolymer (PBDTTHD – DTBTff) was studied and benchmarked against the reference polymer poly-3-hexylthiophene (P3HT). We employed, respectively, four electrode conductivity measurements, Kelvin probe work function measurements, carrier mobility using charge extraction by linearly increasing voltage (CELIV) measurements and diffusion length determination using surface photovoltage measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Charles University, Academy of Sciences of the Czech Republic
Authors: Toušek, J. (Ekstern), Toušková, J. (Ekstern), Remeš, Z. (Ekstern), Chomutová, R. (Ekstern), Čermák, J. (Ekstern), Helgesen, M. (Intern), Carlé, J. E. (Intern), Krebs, F. C. (Intern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: A I P Advances
Volume: 5
Issue number: 12
Article number: 127240
ISSN (Print): 2158-3226
Ratings:
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.32 SJR 0.449 SNIP 0.612
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.457 SNIP 0.619 CiteScore 1.17
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.709 SNIP 0.788 CiteScore 1.38
Web of Science (2014): Indexed yes
Electrical properties and flux performance of composite ceramic hydrogen separation membranes

The electrical properties and hydrogen permeation flux behavior of the all-ceramic protonic/electronic conductor composite BaCe0.2Zr0.7Y0.1O3-δ/Sr0.95Ti0.9Nb0.1O3-δ (BCZY27/STN95: BS27) are evaluated. Conductivity and hydrogen permeability are examined as a function of phase volume ratios. Total conductivities of 0.01-0.06 S cm⁻¹ are obtained in moist (+1% H2O) H2/inert gas from 600-800 °C for 50 volume% STN95. With increasing STN95 content (60 and 70 volume%), conductivity increases by 5-10 times, but displays a semiconductor-type dependence, even at 70 volume% STN95. The conductivity is modeled with an effective medium approach incorporating a term for the heterojunctions between the two phases. Hydrogen fluxes of 0.004-0.008 μmol cm⁻² s⁻¹ are obtained for a 50 volume% STN95 membrane sample (1 mm thickness) at 600-800 °C using dry argon as a sweep gas. Upon adding palladium layers as catalysts more than a five-fold increase is observed in the hydrogen flux, 0.025-0.026 μmol cm⁻² s⁻¹, over the same temperature range. Hydrogen flux is not observed for membranes made from the 60 and 70% STN95 samples.
Electrochemical Impedance Spectroscopy as a Tool for PEMECs Development

Electrochemical reduction of NO with propene in the presence of oxygen on LSCoM/CGO porous cell stacks impregnated with BaO

The electrochemical reduction of NO with propene in the presence of 10 % O2 was studied on a La0.85Sr0.15Co0.03Mn0.97O3-Ce0.9Gd0.1O1.95 11-layer electrochemical reactor. BaO was impregnated into the porous reactor, and electrochemical impedance spectroscopy was used for characterisation in the temperature range of 300–400 °C. They were subjected to different magnitudes of polarisations, and the BaO impregnation was shown to have increased the NO reduction with increasing polarisation in the presence of excess oxygen. At 350 °C, more than 60 % was removed and a current efficiency for the cell stack of up to 30 % was achieved. In the presence of propene, the electrochemical promotion on the NOx conversion decreased and only 13 % was removed. A propene oxidation of 35 % was achieved as the highest at 400 °C. The propene acted as a reducing agent on the barium nitrates and caused a greater reduction of the nitrates and hereby releasing more NO than in the gas without propene. This caused an increase in NO in the outlet gas since not all of it was reduced further to nitrogen. The results indicate that the electrochemical reduction of the nitrates when no propene is present is a surface reaction, whereas the propene enables further reduction of the bulk nitrate.
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.26 SJR 0.662 SNIP 0.721
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.652 SNIP 0.679 CiteScore 2.18
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.834 SNIP 1.009 CiteScore 2.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.735 SNIP 0.926 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.88 SNIP 1.009 CiteScore 2.23
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.871 SNIP 1.002 CiteScore 2.28
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.9 SNIP 0.974
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.851 SNIP 0.908
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.754 SNIP 0.738
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.78 SNIP 0.776
Scopus rating (2006): SJR 0.773 SNIP 0.961
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.63 SNIP 0.84
Scopus rating (2004): SJR 0.53 SNIP 0.766
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.537 SNIP 0.711
Scopus rating (2002): SJR 0.738 SNIP 0.81
Scopus rating (2001): SJR 0.763 SNIP 0.86
Scopus rating (2000): SJR 0.675 SNIP 0.617
Scopus rating (1999): SJR 0.664 SNIP 0.758
Original language: English
HASH(0x3451860), Electric reactors, Electrochemical impedance spectroscopy, Electrolytic reduction, Manganese, Nitrates, Nitrogen, Nitrogen compounds, Oxygen, Polarization, Propylene, Surface reactions, Barium nitrates, Current efficiency, Electrochemical promotion, Electrochemical reactor, Electrochemical reductions, Excess oxygen, Propene oxidation, Temperature range, Reduction
DOIs:
10.1007/s10008-015-2783-1
Source: FindIt
Source-ID: 274160209
Publication: Research - peer-review » Journal article – Annual report year: 2015
Electrochemistry as a Tool for Study, Development and Promotion of Catalytic Reactions

The first two chapters of the dissertation are dedicated to definition of the peculiarities of electrochemical processes and also common features and differences between heterogeneous redox and catalytic reactions and electrochemical reactions. The main common characteristic of heterogeneous catalytic reactions and electrochemical reactions is defined. It is the Fermi level of the catalyst, which is also the electrochemical potential of the electrode. According to the Newns-Anderson theory, Fermi level of catalysts affects (or even define) their activity. The electrochemical potential can be measured and changed by polarization in electrochemical experiment. In Chapter 3 the nature of the electrochemical heterogeneous catalytic reactions is discussed, including the new theory of electrochemical promotion. This theory is based on electrochemical change of the Fermi level of the catalyst. It also states that there are two types of electrochemical promotion: First type is based on change of the Fermi level through the charge of the electric double layer (EDL) between catalyst and its support without electrochemical reaction. This effect was abbreviated as EDLE. Second type is based on change of Fermi level by electrochemical production of promoters, reducing or oxidizing current carriers of the catalyst support (O2-, H+, Na+). This type1 was abbreviated as EEPP. In Chapters 4–7, the results of my research are given as examples of use of electrochemistry as a tool for study, promotion and development of catalysts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Petrushina, I. (Intern)
Number of pages: 187
Publication date: 2015

Publication information
Place of publication: Kgs. Lynby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Electrochemistry_as_a_Tool_for_Study.pdf

Bibliographical note
The defence will take place on Monday, 2 November 2015
Publication: Research › Doctoral thesis – Annual report year: 2015

Electrode Kinetics and Gas Conversion in Solid Oxide Cells

The solid oxide fuel cell (SOFC) converts hydrogen, carbon monoxide and hydrocarbon fuels (directly) into electricity with very high efficiencies and has demonstrated almost comparable performance when operated in reverse mode as a solid oxide electrolysis cell (SOEC). In this case electrical (and thermal) energy is stored as chemical energy of reaction products. To this end, the cells are fed with steam (H2O electrolysis), carbon dioxide (CO2 electrolysis) or a mixture of both (H2O/CO2 co-electrolysis) and of course electrical (ΔG) and thermal (TΔS) energies for the splitting of reactant compounds. Hydrogen, carbon monoxide or both (synthesis gas) are produced at the fuel electrode meanwhile oxygen is produced at the oxygen electrode. In reversible or cyclic mode the solid oxide cell is operated alternatingly as fuel cell or electrolysis cell depending on the needs of the end user.

Upon polarization of the solid oxide cell (SOC) and independent of polarization mode (fuel cell mode or electrolysis mode), the current flowing through the cell is limited by processes such as adsorption and desorption of reactants or products, diffusion through the porous electrodes, activation or charge transfer at the reaction sites, gas conversion at the reaction sites and flow fields and ohmic drop across the electrolyte. These processes occur in both electrodes and often their characteristic frequencies overlap, rendering characterization of a given mechanism particularly challenging. To optimize the SOCs for operation in the different fuels, operation temperature and operation modes it is important to understand the kinetics of the SOC electrodes. This thesis was aimed at understanding the kinetics of the SOC under different operation conditions of temperature, polarization, and fuel mixture. For investigations on full cells, electrochemical impedance spectroscopy and distribution of relaxation times techniques were used to investigate kinetics of the Ni/YSZ fuel electrode in three fuel mixtures – hydrogen/steam and reformate fuels hydrogen/carbon-dioxide and hydrogen/methane/steam. It was found that the kinetics at the fuel electrode were exactly the same in both reformates. This means that chemical equilibrium reactions were much faster than the electrochemical reactions. The electrode displayed slightly faster kinetics in hydrogen/steam fuel than in the reformate fuels.

To minimize the influence of (i) joule heating effects as a result of current flow across the electrolyte, (ii) concentration-related effects like gas diffusion, and (iii) overlapping of the characteristic frequencies of processes, the investigations were extended from full cell geometries to a novel pseudo-three electrode cell geometry with working-electrode areas of ca. 1 mm2 that enabled isolated investigation of the fuel and oxygen electrodes. In a 50:50 H2/H2O fuel mixture, the Ni/8 mol % yttria-stabilized zirconia (Ni/YSZ) fuel electrode showed slower reaction kinetics operating under cathodic polarization than anodic—the same finding had been reported in literature from investigations on full cells whereby together with the local pH2O, substrate diffusion (specifically Knudsen diffusion) was identified as one of the causes of asymmetry between anodic and cathodic mode polarization. Obtained charge-transfer coefficients compared well with
those reported in literature and their evolution with temperature was similar to that reported in literature based on porous Ni/YSZ fuel electrodes. From the two investigated oxygen electrodes, the higher performing (La0.6Sr0.4)0.99Co0.3/Ce0.9Gd0.1O1.95 (LSC/CGO) oxygen electrode showed slower reaction kinetics under cathodic mode operation at 50 mV overvoltage than in anodic mode. The trend was opposite for the lower performing La0.58Sr0.4Co0.2Fe0.8O3 (LSCF) oxygen electrode. However, with decreasing oxygen partial pressure both electrodes displayed increasing asymmetry between anodic and cathodic modes. It could be shown that surface exchange kinetics were the major cause of the decreasing kinetics with decreasing pO2 and that the cathodic mode kinetics were slowed down much more than the anodic branch kinetics thus increasing the asymmetry. Independent of operation mode, commercialization of the SOC technology requires a guarantee of longevity as well as predictability of the SOC performance under desired operation conditions. The performance is generally evaluated through the current/voltage (C/V) curve. As such, a deviation from the expected/predicted performance curve can serve to identify the presence of ageing or an ageing inducing process. A 0-D stationary model was previously developed at the Institut für Angewandte Materialien - Werkstoffe der Elektrotechnik (IAM-WET) in Germany to predict the C/V curve of a SOC for fuel cell operation mode. In this thesis, the applicability of this model was verified for electrolysis mode operation, the model was extended to accommodate temperature changes under polarization in fuel cell and electrolysis mode operation, and the model was further extended to cover operation in reformate fuels H2/H2O/CO/CO2. The latter was accomplished by including a new concentration-related overpotential contribution in the model to account for the CO/CO2 diffusion to the reaction sites as a result of the water gas shift equilibrium reactions.

The long-term stability of the system depends on whether the system is operated solely in fuel-, electrolysis-, reversible or dynamic mode. Optimization of the cells for high performance and/or durability in each of these operation modes requires a thorough understanding of the processes and mechanisms affecting the kinetics and ageing of the systems. In five tests with varying durations between 1000 h and 2500 h the long-term stability of the SOCs was investigated for constant electrolysis, cyclic and dynamic operation modes in a symmetric binary fuel of 50/50 H2/H2O at 800 °C and 700 °C. The SOCs investigated under constant electrolysis mode aged more than those investigated under cyclic mode with the fuel electrode dominating the ageing in constant electrolysis mode and the oxygen electrode dominating that in cyclic mode. During dynamic cycling, the SOCs aged less at 800 °C than at 700 °C. It was observed that for cycles with equal durations in SOEC and SOFC modes whereby the cycle lengths were less than or equal to 2 x 5 h the voltage ageing was almost symmetrical for both SOFC and SOEC modes. For longer cycle lengths SOEC mode voltage ageing was at least double the SOFC mode voltage ageing. This result is consistent with suggestions in literature that intermittent operation of SOCs in fuel cell mode slows down or even reverses SOC ageing that occurs during long-term electrolysis operation. Based on the finding that the fuel electrode dominated the ageing under constant electrolysis operation, it was speculated based on literature, to be caused by precipitation of nickel oxide that had diffused into the 8YSZ matrix of the fuel electrode during sintering. Constant electrolysis operation provided enhanced conditions for the precipitation of the nickel oxide as metallic nickel. Furthermore, Zr, Ni, Y, and O containing nano-particles were found on the Ni particles. In literature during electrolysis of H2O/CO2 under same conditions of temperature and current density nano particles were also found on Ni particles, identified as ZrO2 and attributed the major cause of fuel electrode ageing. In cyclic operation these enhancing conditions were not maintained long-enough for severe nickel precipitation. It is known and was verified that the LSC/CGO electrode is better performing than the LSCF electrode. To compare the stability of these two state-of-the-art (s.t.a.) oxygen electrodes, 1000 h tests under non-polarized or open circuit voltage (OCV) conditions were carried out using symmetric cell geometry. Both electrodes displayed a two-step ageing trend with rapid initial ageing within the first 400 h followed by relaxation to slower ageing rates. The LSCF electrode showed a larger increase in polarization resistance especially within the first 400 h in which it aged by factor 6 faster than the LSC/CGO electrode. The rapid ageing of the LSCF electrode within the first 300 – 400 h of operation has also been reported in literature.

**General information**

State: Published
Organisations: Applied Electrochemistry, Department of Energy Conversion and Storage, Karlsruher Institut für Technologie
Authors: Njodzefon, J. (Intern), Hjelm, J. (Intern), Graves, C. R. (Intern), Weber, A. (Ekstern)
Number of pages: 212
Publication date: 2015

**Publication information**

Place of publication: Roskilde, Denmark
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Electrode Kinetics

**Relations**

Projects:
Electrode Kinetics and Gas Conversion in Solid Oxide Cells
Publication: Research › Ph.D. thesis – Annual report year: 2016
Electrophoresis deposition of Mn$_{1.5}$Co$_{1.5}$O$_4$ on metallic interconnect and interaction with glass-ceramic sealant for solid oxide fuel cells application

Cr-containing stainless steels are widely used as metallic interconnects for SOFCs. Volatile Cr-containing species, which originate from the oxide formed on steel, can poison the cathode material and subsequently cause degradation in the SOFC stack. Mn$_{1.5}$Co$_{1.5}$O$_4$ spinel is one of the most promising coating materials due to its high electrical conductivity, good CTE match with the stainless steel substrate and an excellent chromium retention capability. In this work Mn$_{1.5}$Co$_{1.5}$O$_4$ spinel coatings are deposited on Crofer22APU substrates by cathodic electrophoretic deposition (EPD) followed by sintering at 800-1150 °C in different atmospheres. Dense, continuous and crack free Mn$_{1.5}$Co$_{1.5}$O$_4$ coatings (with thickness ranging from 10 to 40 μm) are obtained on Crofer22APU substrates. Moreover, electrical properties of the coated Crofer22APU alloy are tested up to 2500 h and an excellent compatibility is found between Mn$_{1.5}$Co$_{1.5}$O$_4$ coated Crofer22APU and a new glass-ceramic sealant, after 500 h of thermal tests in air, thus suggesting that the spinel protection layer can effectively act as a barrier to outward diffusion of Cr. [All rights reserved Elsevier].
Electrospinning for Solid Oxide Fuel Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Zhang, W. (. (Intern)
Pages: 61-76
Publication date: 2015

Host publication information
Title of host publication: Electrospinning for Advanced Energy and Environmental Applications
Publisher: CRC Press, Taylor & Francis Group
Editor: Cavaliere, S.
ISBN (Print): 978-1-4822-1767-4
Eliminating degradation in solid oxide electrochemical cells by reversible operation

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Fundamental Electrochemistry
Authors: Graves, C. R. (Intern), Ebbesen, S. D. (Intern), Jensen, S. H. (Intern), Simonsen, S. B. (Intern), Mogensen, M. B. (Intern)
Number of pages: 6
Pages: 239–244
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Materials
Volume: 14
ISSN (Print): 1476-1122
Ratings:
BFI (2018): BFI-level 3
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 23.67 SJR 18.032 SNIP 9.667
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 14.946 SNIP 9.137 CiteScore 23.23
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 16.754 SNIP 9.273 CiteScore 23.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 18.482 SNIP 8.399 CiteScore 21.29
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 17.631 SNIP 7.981 CiteScore 19.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 18.249 SNIP 7.662
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 15.452 SNIP 6.724
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging

The realization of a complete tandem polymer solar cell under ambient conditions using only printing and coating methods on a flexible substrate results in a fully scalable process but also requires accurate control during layer formation to succeed. The serial process where the layers are added one after the other by wet processing leaves plenty of room for error and the process development calls for an analytical technique that enables 3D reconstruction of the layer stack with the possibility to probe thickness, density, and chemistry of the individual layers in the stack. The use of ptychography on a complete 12-layer solar cell stack is presented and it is shown that this technique provides the necessary insight to enable efficient development of inks and processes for the most critical layers in the tandem stack such as the recombination layer where solvent penetration in fully solution processed 12-layer stacks is critical in eleven of the steps.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Imaging and Structural Analysis, Deutsches Elektronen-Synchrotron
Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 5
Issue number: 1
Article number: 1400736
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.124 SNIP 2.045
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.254 SNIP 2.531 CiteScore 14.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.706 SNIP 2.975 CiteScore 15.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.979 SNIP 2.936 CiteScore 13.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
In this article we discuss the synthesis of four new low band-gap co-polymers based on the diketopyrrolopyrrole (DPP) and benzotriazole (BTZ) monomer unit. We demonstrate that the BTZ unit allows for additional solubilizing side-chains on the co-monomer and show that the introduction of a linear side-chain on the DPP-unit leads to an increase in thin-film order and charge-carrier mobility if a sufficiently solubilizing, branched, side chain is attached to the BTZ. We compare two different synthetic routes, direct arylation and Suzuki-polycondensation, by a direct comparison of polymers obtained via the two routes and show that direct arylation produces polymers with lower electrical performance which we attribute to a higher density of chain. Furthermore we demonstrate that a polymer utilizing this design motif and synthesized via Suzuki-polycondensation ((l-C18)-DPP-(b-C17)-BTZ) exhibits exceptionally high and near balanced average electron and hole mobilities >2 cm² V⁻¹ s⁻¹ which are among the highest, robustly extracted mobility values reported for DPP copolymers in a top-gate configuration to date. Our results demonstrate clearly that linear side chain substitution of the DPP unit together with co-monomers that allow for the use of sufficiently long or branched solubilizing side chains can be an attractive design motif for solution processable, high mobility DPP copolymers.
Energy Supply Modelling in Cities, Illustrated Using Data from the Municipality of Sønderborg in Denmark

In the ongoing transition towards a fully sustainable energy system, maximizing the system efficiency and the integration across its sectors while minimizing the costs of the system and carefully prioritizing the usage of energy resources are key issues. Denmark aims at becoming independent of fossil fuels for electricity and heat generation by 2035 and at having a fully renewable energy system by 2050. Harmonized national and regional efforts are required in order to meet these goals. As the majority of the demand for energy services is located in cities, and because the density of energy transmission networks is highest within cities, it is useful to focus on city areas when seeking to optimize the system efficiency, economy and integration. We have performed a case study using data from the Danish municipality of Sønderborg, which has the goal of becoming CO2 neutral by 2029. We have developed and modeled different scenarios for Sønderborg’s energy system in 2029, containing various different energy conversion pathways. These include e.g. biogas production and upgrade using hydrogen from electrolysis, scenarios with biomass gasification and local transport fuel production and scenarios in which gas turbines for reserve electricity generation have been displaced by reversible electrolysis/fuel cell systems. The aim of the case study was to identify if and how new energy conversion technologies can be integrated in the future energy system to meet the demand for energy services in an economical, efficient and sustainable way on a regional scale. The results show that the gas and district-heating systems, along with utility-scale heat pumps, will serve as valuable system integrators for the large amounts of fluctuating electricity supply from wind and PV. The overall system efficiency can be enhanced by supplying surplus process heat to the district-heating network and by using electrolysis to produce hydrogen for upgrading of biomass-derived gases. The results also pinpoint the importance of prioritizing biomass for the production of synthetic hydrocarbon transport fuels rather than for heat and power generation. The work was carried out using the Sifre energy systems analysis software developed by Energinet.dk (the Danish electricity and gas TSO). It is a linear optimization model that seeks a least-cost solution for the hour-by-hour operation of the specified energy system. The work was carried out as part of CITIES, funded by Innovation Fund Denmark.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Energinet.dk
Authors: Sveinbjörnsson, D. Þ. (Intern), Algren, L. (Ekstern), Bavnhøj Hansen, A. (Ekstern), Pedersen, A. S. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 117919875
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Enhanced reducibility and electronic conductivity of Nb or W doped Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ – $\delta$

The transport and theromechanical properties of acceptor (Gd) and donor (Nb or W) co-doped ceria were investigated. The solubility limit of Nb in Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ – $\delta$ (CGO10) exceeds 4 at.%, whereas that of W is approximately 2 at.%. Both the thermal and stoichiometric expansion coefficients are decreased relative to that of CGO10. Charge compensation of the donor dopants takes place primarily by annihilation of oxide ion vacancies, and a sharp decrease in ionic mobility is observed upon Nb or W doping of CGO10. On the other hand, the n-type electronic conductivity, associated with the reduction of Ce$^{4+}$, increases upon doping with Nb or W, due to enhanced reducibility of cerium. This is beneficial for applications where electronic conductivity is also required, like oxygen permeation membranes. Modeling shows that 4
at.% Nb or W doped CGO10 will deliver higher oxygen fluxes than CGO10, due to the enhanced electronic conductivity and despite the reduced ionic conductivity.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Ceramic Engineering & Science, Mixed Conductors
Authors: Chatzichristodoulou, C. (Intern), Ricote, S. (Intern), Foghmoes, S. P. V. (Intern), Glasscock, J. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 6
Pages: 51-56
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Solid State Ionics
Volume: 269
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.055 SNIP 1.258 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.383 SNIP 1.621 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.459 SNIP 1.503
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.507 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.516 SNIP 1.621
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.301 SNIP 1.392
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.235 SNIP 1.543
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.088 SNIP 1.431
Enhancement of the chemical stability in confined δ-Bi₂O₃

Bismuth-oxide-based materials are the building blocks for modern ferroelectrics, multiferoics, gas sensors, light photocatalysts and fuel cells. Although the cubic fluorite δ-phase of bismuth oxide (δ-Bi₂O₃) exhibits the highest conductivity of known solid-state oxygen ion conductors, its instability prevents use at low temperature. Here we demonstrate the possibility of stabilizing δ-Bi₂O₃ using highly coherent interfaces of alternating layers of Er₂O₃-stabilized δ-Bi₂O₃ and Gd₂O₃-doped CeO₂. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for Bi₂O₃-based materials, is achieved. Even more interestingly, at low oxygen partial pressure the layered material shows anomalous high conductivity, equal or superior to pure δ-Bi₂O₃ in air. This suggests a strategy to design and stabilize new materials that are comprised of intrinsically unstable but high-performing component materials.

General information
State: Published
Number of pages: 5
Pages: 500-504
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Materials
Volume: 14
Issue number: 5
ISSN (Print): 1476-1122
Ratings:
BFI (2018): BFI-level 3
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 23.67 SJR 18.032 SNIP 9.667
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
Enhancing hybrid direct carbon fuel cell anode performance using Ag$_2$O

A hybrid-direct carbon fuel cell (HDCFC), consisting of a molten slurry of solid carbon black and (Li-K)$_2$CO$_3$ added to the anode chamber of a solid oxide fuel cell, was characterized using current-potential-power density curves, electrochemical impedance spectroscopy, and cyclic voltammetry. Two types of experimental setups were employed in this study, an anode-supported full cell configuration (two electrodes, two atmospheres setup) and a 3-electrode electrolyte-supported half-cell setup (single atmosphere). Anode processes with and without catalysts were investigated as a function of temperature (700-800 °C) and anode sweep gas (N$_2$, 4-100% CO$_2$ in N$_2$-CO$_2$). It was shown that the addition of silver based catalysts (Ag, Ag$_2$O, Ag$_2$CO$_3$) into the carbon-carbonate slurry enhanced the performance of the HDCFC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Deleebeeck, L. (Intern), Ippolito, D. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 18
Pages: 222-239
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 152
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.651 SNIP 1.592 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.621 SNIP 1.803 CiteScore 4.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.691 SNIP 1.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.536 SNIP 1.625
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.533 SNIP 1.47
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.563 SNIP 1.595
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.534 SNIP 1.736
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.481 SNIP 1.533
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.365 SNIP 1.581
Scopus rating (2003): SJR 1.628 SNIP 1.526
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.644 SNIP 1.459
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.319 SNIP 1.408
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.009 SNIP 1.168
Web of Science (2000): Indexed yes
Environmental benefits of parking-integrated photovoltaics: A 222kWp experience

The life cycle assessment of a grid-connected, parking integrated, 222kWp cadmium telluride photovoltaic system has been performed. The system was built at the University of Murcia and has been monitored for 2.5 years (sampling data every 5 min). The detailed material inventory, the energy embedded in the system, the energy payback time, and the energy return factor of the facility have been obtained and are 6.31 TJ equivalent primary energy, 2.06 and 12.16 years, respectively. The average performance ratio is 0.8 with a slight monthly variation. Additionally, the environmental benefits of the architectural integration (in this case parking integration) have been quantified using a standard methodology for the calculation of several environmental parameters. Finally, the environmental benefits of renewable energy generation because of the savings of producing the same amount of electricity by the Spanish grid system have been assessed. © 2013 John Wiley & Sons, Ltd.
Environmental impacts of electricity generation at global, regional and national scales in 1980–2011: What can we learn for future energy planning?

The generation of electricity has been known to cause important damages to ecosystems and human health. The recognition of the global challenges posed by climate change and energy security has guided several countries to change their electricity policies over the past decades. However, have such changes entailed reduced or increased environmental impacts? Are there any identifiable patterns that could serve for steering future energy planning? To address these questions, we applied life cycle assessment to quantify a whole spectrum of environmental impacts caused by electricity generation in 199 countries for the period 1980–2011, with national differentiation of energy sources and, wherever possible, technology efficiencies. The results show that (i) environmental impact burden-shifting has occurred in the past for several countries as a result of national policies, (ii) all environmental impacts have globally increased since 1980 but with faster increase rates over the last decade, and (iii) important variations exist in the impact trends across countries and across impact categories. Our findings therefore demonstrate the need for integrating quantitative assessments of all relevant environmental impacts associated with foreseen energy systems when identifying the most sustainable energy pathways. We provide recommendations on the use of life cycle assessment for such purposes with a strong focus on application at the country level so that it can directly support national energy policy-making.
Environmental TEM study of the dynamic nanoscaled morphology of NiO/YSZ during reduction

The reduction of a metal oxide is often a critical preparation step for activating catalytic behaviour. This study addresses the reduction process of NiO in pure form and in a composite of NiO/yttria-stabilized zirconia (YSZ) in hydrogen relevant for solid oxide electrochemical cells by comparing results from environmental transmission electron microscopy (ETEM) with thermogravimetric analysis (TGA). The temperature dependent reduction profiles obtained from TGA confirm an inhibitive effect from YSZ on the NiO reduction. The ETEM images show the growth of Ni in decaying NiO and reveal the nanoscale morphological changes such as pore formation in NiO above 280°C and densification and collapse of the pore structures above 400°C. The accelerated Ni front in NiO illustrates the auto catalysis of the reaction. A rapid temperature ramping from room temperature to 780°C in hydrogen in 1 second resulted in immediate morphological changes at the nanoscale from dense NiO to dense Ni. The analysis suggests that the inhibitive effect of YSZ on the NiO reduction reaction is not due to a direct local interaction between YSZ and NiO, but instead due to gas and/or mass transport limitations.© 2014 Elsevier B.V. All rights reserved.
Nickel oxide reduction, NiO, YSZ, SOFC, SOEC, In situ TEM, ETEM, Autocatalysis
Er der vedvarende energi nok til os alle?: om brændselsceller og elektrolyseceller til effektiv energikonvertering

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Hauch, A. (Intern)
Number of pages: 29
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Brændselsceller_og_elektrolyseceller_DanskNaturvidenskabsfestival_AnneHauch_September26th2014.pdf

Relations
Activities:
Er der vedvarende energi nok til os alle?: Om brændselsceller og elektrolyseceller til effektiv energikonvertering
Publication: Research › Sound/Visual production (digital) – Annual report year: 2015

Erratum: In Situ Studies of Fe⁴⁺ Stability in β-Li₃Fe₂(PO₄)₃ Cathodes for Li Ion Batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Neutrons and X-rays for Materials Physics, Applied Electrochemistry, Fundamental Electrochemistry
Authors: Christiansen, A. S. (Intern), Johnsen, R. E. (Intern), Norby, P. (Intern), Frandsen, C. (Intern), Mørup, S. (Intern), Jensen, S. H. (Intern), Kammer Hansen, K. (Intern), Holtappels, P. (Intern)
Pages: X11-X11
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Journal
Volume: 162
Issue number: 6
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.037 SNIP 1 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
Experimental Studies with an Active Magnetic Regenerating Refrigerator

Experimental results for an active magnetic regenerator (AMR) are presented. The focus is on whether or not it pays off to partly substitute soft magnetic material with non-magnetic insulation in a flux-conducting core in the magnet system. Such a substitution reduces losses due to heat conduction and eddy currents, but also reduces the magnetic field. Two different cores were tested in the AMR system with different cooling loads and it is shown, that in the present case, replacing half of the iron with insulation lead to an average reduction in temperature span of 14%, but also a small decrease in COP, hence the substitution did not pay off. Furthermore, it is shown experimentally, that small imbalances in the heat transfer fluid flow greatly influence the system performance. A reduction of these imbalances through valve adjustments resulted in an increase in the temperature span from approximately 16 K to 27.3 K.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrophysical materials
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

The discovery of two-dimensional electron gases (2DEGs) at the interface between two insulating complex oxides, such as LaAlO3 (LAO) or gamma-Al2O3 (GAO) epitaxially grown on SrTiO3 (STO), provides an opportunity for developing all-oxide electronic devices. These 2DEGs at complex oxide interfaces involve many-body interactions and give rise to a rich set of phenomena, for example, superconductivity, magnetism, tunable metal-insulator transitions, and phase separation. However, large enhancement of the interfacial electron mobility remains a major and long-standing challenge for fundamental as well as applied research of complex oxides. Here, we inserted a single unit cell insulating layer of polar La1-xSr1+xMnO3 (x=0, 1/8, and 1/3) at the interface between disordered LaAlO3 and crystalline SrTiO3 created at room temperature. We find that the electron mobility of the interfacial 2DEG is enhanced by more than two orders of magnitude. Our in-situ and resonant x-ray spectroscopic in addition to transmission electron microscopy results indicate that the manganite layer undergoes unambiguous electronic reconstruction and leads to modulation doping of such atomically engineered complex oxide heterointerfaces. At low temperatures, the modulation-doped 2DEG exhibits clear Shubnikov-de Haas oscillations and the initial manifestation of the quantum Hall effect, demonstrating an unprecedented high-mobility and low electron density oxide 2DEG system. These findings open new avenues for oxide electronics.
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen
Number of pages: 2
Publication date: 2015
Event: Abstract from 22nd International Workshop on Oxide Electronics, Paris, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Extreme_mobility_enhancement.pdf
DOI: 10.1038/nmat4303
Source: PublicationPreSubmission
Source-ID: 108165813
Publication: Research - peer-review › Journal article – Annual report year: 2015

Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen
Number of pages: 1
Publication date: 2015
Event: Poster session presented at E-MRS 2015 Fall meeting, Warsaw, Poland.
Main Research Area: Technical/natural sciences
Electronic versions:
Extreme_mobility_enhancement_poster.pdf
Publication: Research › Poster – Annual report year: 2015

Fabrication and performance of a tubular ceria based oxygen transport membrane on a low cost MgO support
A 30 μm thin-film tubular CGO (Ce0.9Gd0.1O1.95−δ) membrane with catalytic layers on both sides has been prepared by dip-coating on a low cost, porous magnesium oxide (MgO) support. The MgO support was fabricated through a thermoplastic extrusion process. Support, thin membrane and catalytic layers were sintered in individual steps at temperatures between 1250 and 1300 °C to achieve a controlled removal of binder and organic additives and to obtain the desired, defect free microstructure. The prepared asymmetric tubular CGO membrane has been tested at elevated temperatures (up to 900 °C) using atmospheric air and N2, H2 for the feed and sweep side respectively. The oxygen permeation was 4 N ml min−1 cm−2 at 850 °C using H2 on one side and air on the other side.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Swiss Federal Laboratories for Materials Testing and Research
Authors: Kothanda Ramachandran, D. (Intern), Søgaard, M. (Intern), Clemens, F. (Ekstern), Gurauskis, J. (Intern), Kaiser, A. (Intern)
Pages: 422–430
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: Separation and Purification Technology
Volume: 147
ISSN (Print): 1383-5866
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.023 SNIP 1.394
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.078 SNIP 1.504 CiteScore 3.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.257 SNIP 1.54 CiteScore 3.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.325 SNIP 1.678 CiteScore 3.62
ISI indexed (2013): ISI indexed yes
Nanostructured materials have attracted incredible interest during the recent years for a large variety of applications. In heterogeneous catalysis the use of nano-sized catalytic materials is expected to significantly impact the performances of materials as consequence of their large surface-to-volume ratios [1]. The “nanomaterial” approach enables to achieve structures with incredible large exposed surface area. When nanofibers are used as nano-catalysts, the further advantage of a quite open porous structure is further achieved. In this work, nanomaterial approach was adopted to fabricate nano-catalysts for the removal of the NOx in exhausts via the NH3 Selective Catalytic Reduction method (SCR). The state-of-art system WO3-V2O5 was incorporated into TiO2 ceramic nanofibers through combination of electrospinning and sol-gel process. Catalytic functionalized nanofibers were characterized using SEM, TEM, EDX, BET, XRD, to analyze fiber diameter, morphology, composition, specific surface area, crystallization phases of TiO2 functionalized, atomic percentage of elements in fiber respectively. Catalytic activity was also measured.

Fabrication of doped Titania (TiO2) nano-catalysts in the shape of nanofibers
Nanostructured materials have attracted incredible interest during the recent years for a large variety of applications. In heterogeneous catalysis the use of nano-sized catalytic materials is expected to significantly impact the performances of materials as consequence of their large surface-to-volume ratios [1]. The “nanomaterial” approach enables to achieve structures with incredible large exposed surface area. When nanofibers are used as nano-catalysts, the further advantage of a quite open porous structure is further achieved. In this work, nanomaterial approach was adopted to fabricate nano-catalysts for the removal of the NOx in exhausts via the NH3 Selective Catalytic Reduction method (SCR). The state-of-art system WO3-V2O5 was incorporated into TiO2 ceramic nanofibers through combination of electrospinning and sol-gel process. Catalytic functionalized nanofibers were characterized using SEM, TEM, EDX, BET, XRD, to analyze fiber diameter, morphology, composition, specific surface area, crystallization phases of TiO2 functionalized, atomic percentage of elements in fiber respectively. Catalytic activity was also measured.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Technical University of Denmark
Authors: Marani, D. (Intern), Silva, R. H. (Ekstern), Zhang, W. (. (Intern), Werchmeister, R. M. L. (Intern), Kammer Hansen, K. (Intern), Esposito, V. (Intern)
Publication date: 2015
Event: Abstract from 1st Annual World Congress of Smart Materials 2015, Busan, Korea, Republic of.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Fabrication of Ni-5 at. %W Long Tapes with CeO₂ Buffer Layer by Reel-to-Reel Method

A 10-m-long homemade textured Ni-5at.%W (Ni5W) long tape with a CeO₂ buffer layer has been prepared successfully by means of rolling-assisted biaxially textured substrate (RABiTS) route followed by a chemical solution deposition method in a reel-to-reel manner. Globally, the Ni5W substrate and CeO₂ film exhibit high homogeneity in terms of biaxial texture over the tape. The average values of full width at half maximum of in-plane and out-of-plane texture are 7.2° and 6.1° in Ni5W substrate, 7.6° and 6.1° in CeO₂ buffer layer, respectively, all of those with a small standard deviation. On a microlevel, the CeO₂ film epitaxially grows well on top of the Ni5W tape. A continuous, smooth, and crack-free morphology was observed on the CeO₂ film and the fraction of low-angle grain boundaries (≤ 10°) is about 98 %. This process is a potential possibility for producing long-length textured CeO₂/Ni5W tapes for coated conductors with a low cost.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Beijing University of Technology
Authors: Ma, L. (Ekstern), Tian, H. (Ekstern), Yue, Z. (Intern), Gao, M. (Ekstern), Suo, H. (Ekstern), Grivel, J. (Intern)
Number of pages: 7
Pages: 2959-2965
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Superconductivity and Novel Magnetism
Volume: 28
Issue number: 10
ISSN (Print): 1557-1939
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.91 SJR 0.34 SNIP 0.546
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.325 SNIP 0.556 CiteScore 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.384 SNIP 0.637 CiteScore 0.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.326 SNIP 0.666 CiteScore 0.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.42 SNIP 0.51 CiteScore 0.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.443 SNIP 0.436 CiteScore 0.71
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.665 SNIP 0.41
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.481 SNIP 0.379
Fabrication of porous 3-YSZ turbular supports for oxygen transport membranes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Bjørnetun Haugen, A. (Intern), Gurauskis, J. (Intern), Ovtar, S. (Intern), Hendriksen, P. V. (Intern), Kaiser, A. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Summer school on Ionic and protonic conducting ceramic membranes for green energy applications, Valencia, Spain.
Main Research Area: Technical/natural sciences
Electronic versions:
Fabrication_of_porous.pdf

Bibliographical note
Poster presentation
Source: PublicationPreSubmission
Source-ID: 118022937
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Fabrication of thin yttria-stabilized-zirconia dense electrolyte layers by inkjet printing for high performing solid oxide fuel cells

In this work, we present how a low-cost HP Deskjet 1000 inkjet printer was used to fabricate a 1.2 mm thin, dense and gas tight 16 cm² solid oxide fuel cells (SOFC) electrolyte. The electrolyte was printed using an ink made of highly diluted (<4 vol.%) nanometric yttria stabilized zirconia (YSZ) powders (50 nm in size) in an aqueous medium. The ink was designed to be a highly dispersed, long term stable colloidal suspension, with optimal printability characteristics. The electrolyte was made by a multiple printing procedure, which ensures coverage of the several flaws occurring in a single printing pass. Together with an optimized sintering procedure this resulted in good adhesion and densification of the electrolyte. The SOFC exhibited a close-to-theoretical open circuit voltage and a remarkable peak power density above 1.5 W cm⁻² at 800 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Fundamental Electrochemistry, Mixed Conductors
Pages: 89-95
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Fast mass interdiffusion in ceria/alumina composite
Gadolinium-doped ceria (CGO) presents unique processes at low oxygen partial pressure (pO2 < 10^-12 atm) and low temperatures (T > 800 °C) such as faster mass diffusion, which are not observed in conventional sintering under ambient air conditions. In CGO/Al2O3 composites the resulting effects driven by such mass diffusion are low viscosity flows and high reactivity between phases, indicated by the formation of CeAlO3. This reaction is promoted by the high content of oxygen defects and the chemical reduction of Ce4+ cations to Ce3+ in CGO/Al2O3 composites under low temperature and low pO2. In this work, a comparison is made between sintering CGO/Al2O3 under ambient air conditions and under low pO2, focusing on densification, viscosity and the evolution of the microstructure.

Fe3C-based oxygen reduction catalysts: synthesis, hollow spherical structures and applications in fuel cells
We present a detailed study of a novel Fe3C-based spherical catalyst with respect to synthetic parameters, nanostructure formation, ORR active sites and fuel cell demonstration. The catalyst is synthesized by high temperature autoclave pyrolysis using decomposing precursors. Below 500 °C, melamine-rich microspheres are first developed with uniformly dispersed amorphous Fe species. During the following pyrolysis at temperatures from 600 to 660 °C, a small amount of Fe3C phase with possible Fe-Nx/Cactive sites are formed, however, with moderate catalytic activity, likely limited by the low conductivity of the catalyst. At high pyrolytic temperatures of 700–800 °C, simultaneous formation of Fe3C nanoparticles and encasing graphitic layers occur within the morphological confinement of the microspheres. With negligible surface nitrogen or iron functionality, the thus-obtained catalysts exhibit superior ORR activity and stability. A new ORR active phase of Fe3C nanoparticles encapsulated by thin graphitic layers is proposed. The activity and durability of the catalysts are demonstrated in both Nafion-based low temperature and acid doped polybenzimidazole-based high
temperature proton exchange membrane fuel cells.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Imaging and Structural Analysis, Institut National de la Recherche Scientifique, Chinese Academy of Sciences
Pages: 1752-1760
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Materials Chemistry A
Volume: 3
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
DOIs:
10.1039/c4ta03986f
Source: PublicationPreSubmission
Source-ID: 103528884
Publication: Research - peer-review › Journal article – Annual report year: 2014

**Fine structure of modal focusing effect in a three dimensional plasma-sheath-lens formed by disk electrodes**
Modal and discrete focusing effects associated with three-dimensional plasma-sheath-lenses show promising potential for applications in ion beam extraction, mass spectrometry, plasma diagnostics and for basic studies of plasma sheath. The ion focusing properties can be adjusted by controlling the geometrical structure of the plasma-sheath-lens and plasma parameters. The positive and negative ion kinetics within the plasma-sheath-lens are investigated both experimentally and theoretically and a modal focusing ring is identified on the surface of disk electrodes. The focusing ring is very sensitive to the sheath thickness and can be used to monitor very small changes in plasma parameters. Three dimensional simulations are found to be in very good agreement with experiments.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Nagoya University
Authors: Stamate, E. (Intern), Yamaguchi, M. (Ekstern)
Number of pages: 4
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 107
Issue number: 9
Article number: 094106
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.132 SNIP 0.996
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.799 SNIP 1.462 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.149 SNIP 1.652 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.554 SNIP 1.754 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.805 SNIP 1.94 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.926 SNIP 1.789
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.857 SNIP 1.848
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.934 SNIP 1.83
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.039 SNIP 1.913
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.457 SNIP 2.288
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.709 SNIP 2.382
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.904 SNIP 2.38
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.765 SNIP 2.27
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 3.917 SNIP 2.365
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 4.111 SNIP 2.212
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 4.277 SNIP 2.013
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 4.35 SNIP 2.11
Original language: English
Electronic versions:
Fine_structure_of_modal_focusing_effect.pdf
First principles investigation of the activity of thin film Pt, Pd and Au surface alloys for oxygen reduction

Further advances in fuel cell technologies are hampered by kinetic limitations associated with the sluggish cathodic oxygen reduction reaction. We have investigated a range of different formulations of binary and ternary Pt, Pd and Au thin films as electrocatalysts for oxygen reduction. The most active binary thin films are near-surface alloys of Pt with subsurface Pd and certain PdAu and PtAu thin films with surface and/or subsurface Au. The most active ternary thin films are with pure metal Pt or Pd skins with some degree of Au in the surface and/or subsurface layer and the near-surface alloys of Au with mixed Pt/Pd skins. The activity of the binary and ternary catalysts is explained through weakening of the OH binding energy caused by solute elements. However, given the low alloy formation energies it may be difficult to tune and retain the composition under operating conditions. This is particularly challenging for alloys containing Au due to a high propensity of Au to segregate to the surface. We also show that once Au is on the surface it will diffuse to defect sites, explaining why small amounts of Au retard dissolution of Pt nanoparticles. For the PtPd thin films there is no pronounced driving force for surface segregation, diffusion to defects or surface self-assembling. On the basis of stability and activity analysis we conclude that the near surface alloy of Pd in Pt and some PdAu binary and PtPdAu ternary thin films with a controlled amount of Au are the best catalysts for oxygen reduction.
Flexible sample environment for high resolution neutron imaging at high temperatures in controlled atmosphere

High material penetration by neutrons allows for experiments using sophisticated sample environments providing complex conditions. Thus, neutron imaging holds potential for performing in situ nondestructive measurements on large samples or even full technological systems, which are not possible with any other technique. This paper presents a new sample environment for in situ high resolution neutron imaging experiments at temperatures from room temperature up to 1100 °C and/or using controllable flow of reactive atmospheres. The design also offers the possibility to directly combine imaging with diffraction measurements. Design, special features, and specification of the furnace are described. In addition, examples of experiments successfully performed at various neutron facilities with the furnace, as well as examples of possible applications are presented. This covers a broad field of research from fundamental to technological investigations of various types of materials and components. © 2015 AIP Publishing LLC.
Fullerene alloy formation and the benefits for efficient printing of ternary blend organic solar cells

Composition average dependent properties for blends of the conjugated polymer P3HT and the fullerenes [60]PCBM, [60]ICBA and their mixtures were studied using cross-polarization magic-angle-spinning solid-state NMR techniques. We found that the blended fullerenes form an alloy and that when mixed with a third polymer component, the system exhibits pseudo-binary phase behaviour instead of the expected ternary phase behaviour. Our results experimentally confirm the earlier hypothesis that the unexpected composition average dependent IV-behaviour for these supposed ternary mixtures are indeed due to them behaving as pseudo-binary mixtures due to alloying of the fullerene components. This finding has vast implications for the understanding of polymer–fullerene mixtures and quite certainly also their application in organic solar cells where performance hinges critically on the blend behaviour which is also investigated in this study.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Aarhus University, University of Southern California
Authors: Angmo, D. (Intern), Bjerring, M. (Ekstern), Nielsen, N. C. (Ekstern), Thompson, B. C. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 8
Pages: 5541-5548
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry C
Volume: 3
Issue number: 21
ISSN (Print): 2050-7526
Ratings:
BFI (2018); BFI-level 2
BFI (2017); BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016); BFI-level 1
Scopus rating (2016); CiteScore 5.14 SJR 1.806 SNIP 1.28
Web of Science (2016): Indexed yes
BFI (2015); BFI-level 1
Scopus rating (2015); SJR 1.751 SNIP 1.577 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014); BFI-level 1
Scopus rating (2014); SJR 1.505 SNIP 1.36 CiteScore 4.64
Functional Analysis of Battery Management Systems using Multi-Cell HIL Simulator

Developers and manufacturers of Battery Management Systems (BMSs) require extensive testing of controller HW and SW, such as analog front-end (AFE) and performance of generated control code. In comparison with tests conducted on real batteries, tests conducted on hardware-in-the-loop (HIL) simulator may be more costant time effective, easier to reproduce and safer beyond the normal range of operation, especially at early stages in the development process or during fault simulation. In this paper a li-ion battery (LIB) electro-thermal multicell model coupled with an aging model is designed, characterized and validated based on experimental data, converted to C code and emulated in real-time with a dSpace HIL simulator. The BMS to be tested interacts with the emulated battery pack as if it was managing a real battery pack. BMS functions such as protection, measuring of current, voltage and temperature or balancing are tested on real-time experiments.

Functionally Graded Ceramics Fabricated with Side-by-Side Tape Casting for Use in Magnetic Refrigeration

Functionally graded ceramic tapes have been fabricated by a side-by-side tape casting technique. This study shows the possibility and describes the main principles of adjacent coflow of slurries resulting in formation of thin plates of graded ceramic material. Results showed that the small variations of solvent and binder system concentrations have a substantial effect on slurry viscosity. Varying these parameters showed that side-by-side tape casting with a well-defined interface area is possible for slurries with viscosities above 3500 mPa s at a casting shear rate of 3.3 s⁻¹. As it was expected, the choice of de-bindering and sintering regimes significantly influences crack formation, and a three-step heating programme was found to result in tapes of the highest quality. The interface regions of green graded tapes were investigated structurally by scanning electron microscopy; for a distinct identification of the interface region and analysing the degree of cross-interface diffusion, the isothermal entropy change was measured by a vibrating sample magnetometer as the magnetic transition temperature (Curie temperature) is very sensitive to the dopant level in ceramics. Also the purpose of developing this graded ceramic tape casting was applications of these specific magnetocaloric properties within the magnetic refrigeration technology.
Fundamental electrochemistry: general discussion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry
Number of pages: 36
Pages: 177-212
Publication date: 2015
Main Research Area: Technical/natural sciences
Fundamental mechanisms in Li-air battery electrochemistry
The lithium-air (or Li-O2) batteries have received wide attention as an enabling technology for a mass market entry of electric vehicles due to a potential capacity much higher than current Li-ion technology. The technology is a relatively new battery concept proposed in 1996, and the current research still focuses on developing an understanding of the reactions inside the battery. This thesis is dedicated to increase this understanding and use the knowledge to improve the performance of the battery, and the work span from detailed investigation of the atom positions to the proposal of a system used to manage a full size electric vehicle battery. An automated differential electrochemical mass spectrometer (DEMS) was built to investigate the relationship between current and the consumption and release of gases, which is important to identify and quantify degradation reactions. The setup was used to characterize our carbon-based reference system as well as new ionic liquid-based electrolytes. Electrochemical impedance spectroscopy (EIS) has been used extensively to describe reaction mechanisms inside the battery; the origin of the measured overpotentials; and the onset potential for electrochemical degradation. It was confirmed that the rapid potential loss near the end of discharge could be explained by
an increase in the charge transport resistance; that the initial Li2O2 oxidation at 3.05 V was blocked by the formation of an
SEI layer; and that the voltage increase during charge was primarily due to the formation of a mixed potential between
competing oxidation reactions needed to maintain a constant current. The knowledge about impedance spectroscopy was
used to propose and investigate a novel battery management tool to estimate the state of charge and the state of health of
a Li-O2 battery system better than any other method available. Finally, calculations were made to support that an open
system configuration is a realistic option in terms of air purification, if H2O and CO2 levels at 1 ppm are allowed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Haldor Topsoe AS
Authors: Højberg, J. (Intern), Vegge, T. (Intern), Norby, P. (Intern), Johansen, K. (Ekstern)
Number of pages: 199
Publication date: 2015

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD_Thesis_20150520_rev1_til_Orbit.pdf
Publication: Research › Ph.D. thesis – Annual report year: 2015

Graphene oxide and hyperbranched polymer-toughened hydrogels with improved absorption properties and durability
Hyperbranched polymers or/and graphene oxide nanosheets were used to synthesize poly(acrylic acid)-based hybrid
hydrogels with high water absorption ability, excellent mechanical properties, and environmental remediation abilities
through a novel one-step, cost-effective, and environmentally friendly method. The combination of hyperbranched
polymers and graphene oxide nanosheets had synergistic effects on the final hybrid hydrogel, especially on the
mechanical behaviors of the hydrogels, with Young's modulus, tensile strength at break and elongation at break increasing
by 69, 308, and 848 %, respectively, while the other properties remained similar to those of pure poly(acrylic acid). The
proposed enhancement mechanism is also discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Flinders University,
South China University of Technology, University of South Australia
Authors: Yu, Y. (Ekstern), De Andrade, L. C. X. (Ekstern), Fang, L. (Ekstern), Ma, J. (Ekstern), Zhang, W. (. (Intern),
Tang, Y. (Ekstern)
Number of pages: 10
Pages: 3457-3466
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Science
Volume: 50
Issue number: 9
ISSN (Print): 0022-2461
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.762 SNIP 1.064
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.811 SNIP 1.081 CiteScore 2.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.985 SNIP 1.431 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.933 SNIP 1.472 CiteScore 2.36
Growth of Highly Epitaxial YBa$_2$Cu$_3$O$_{7-δ}$ Films from a Simple Propionate-Based Solution

Intensive investigations have been conducted to develop epitaxial oxide thin films with superior electromagnetic performance by low-cost chemical solution deposition routes. In this paper, a novel propionate-based precursor solution without involving any other additive was proposed and employed to grow superconducting YBa$_2$Cu$_3$O$_7$-5 (YBCO) films on LaAlO$_3$ (LAO) single crystals. The precursor solutions are stable with a long shelf life of up to several months. Since the primary compositions are propionates after evaporating the solvent, the toxic reagents and evolved gases during solution synthesis and heat treatment can be eliminated completely. In this process, rapid pyrolysis and high conversation rate can also be achieved during growth of YBCO films in comparison with the conventional trifluoroacetate metal organic deposition routes. Remarkably, a 210 nm YBCO film exhibits high superconducting performance with a $J_c$ value of 3.7 MA/cm$^2$ at 77 K, self-field. Nucleation and growth behaviors in the chemical solution process have also been studied. It
is revealed that the amount of liquid phase (Ba-Cu-O) is sufficient through the entire thickness within a very short time at high growth temperatures, which results in pronounced densification and fast conversion of the YBCO phase.
H/D isotope effects in high temperature proton conductors

The atomic mass ratio of ca. 2 between deuterium and hydrogen is the highest for any pair of stable isotopes and results in significant and measurable H/D isotope effects in high temperature proton conductors containing these species. This paper discusses H/D isotope effects manifested in O-H/O-D vibration frequencies, the mobility of H\(^+\)/D\(^+\) carriers, the kinetics of the electrochemical oxidation of H\(_2\)/D\(_2\), the solubilities of H\(_2\)O/D\(_2\)O and, finally, the spontaneous electromotive force that appears across H\(_2\)/D\(_2\) cells with proton conducting electrolytes. Comparable work on tritium-exchanged materials is also discussed. The results highlight the usefulness of isotope effects in the study of high temperature proton conductors.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Twente
Authors: Bonanos, N. (Intern), Huijser, A. (Ekstern), Poulsen, F. W. (Intern)
Number of pages: 5
Pages: 9-13
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 275
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
High-$J_c$ YBa$_2$Cu$_3$O$_{7-x}$-Ag superconducting thin films synthesized through a fluorine-free MOD method

Obtaining a high critical current density ($J_c$) remains the main challenge in developing fluorine-free metal organic deposition (MOD) methods to fabricate YBCO superconducting thin films. Silver addition was used to raise the $J_c$ values in this research work. By reacting with propionic acid and ammonia, AgNO$_3$ was initially mixed with YBCO carboxylate precursors dissolved in methanol. High-temperature in situ XRD measurements on the YBCO-Ag powders revealed that silver addition lowers the incongruent melting temperature of YBCO to 760°C and resulted in a smooth surface morphology of the YBCO films at a temperature as low as 760°C. Grain growth and intergranular conductivity were also found to be improved by silver doping. After annealing under optimized conditions, a high $J_c$ of 4.6MA/cm$^2$ was obtained in a YBCO-Ag thin film with 10 wt% Ag.

General information
Highly Confined Electronic and Ionic Conduction in Oxide Heterostructures

The conductance confined at the interface of complex oxide heterostructures provides new opportunities to explore nanoelectronic as well as nanionic devices. In this talk I will present our recent results both on ionic and electronic conductivity at different heterostructures systems. In the first part of my talk I will show some of our resent results that we demonstrated the possibility of stabilizing δ-Bi2O3 using highly coherent interfaces of alternating layers. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for Bi2O3-based materials, is achieved[1]. These confined heterostructures provide a playground not only for new high ionic conductivity phenomena that are sufficiently stable but also uncover a large variety of possible technological perspectives. At the second part, I will discuss and show our recent results of high mobile samples realized by, interface confined redox reactions[2], strain induced polarization[3]and modulation doping at complex oxide interfaces. This collection of samples offers unique opportunities for a wide range of rich world of mesoscopic physics. [1] S. Sanne et al. "Enhancement of the chemical stability in confined δ-Bi2O3". Nature Materials (2015) doi:10.1038/nmat4266 [2] Y. Z. Chen et al. "A high-mobility two-dimensional electron gas at the spinel/perovskite interface of γ-Al2O3/SrTiO3". Nature Commun. 4, 1371 (2013) [3] Y. Z. Chen et al. "Creation of High Mobility Two-Dimensional Electron Gases via Strain Induced Polarization at an Otherwise Nonpolar Complex Oxide Interface" Nano Letters. 3774-3778 (2015) 10.1021/nl504622w

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Pryds, N. (Intern)
Number of pages: 1
Pages: 1266
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-02
Issue number: 36
ISSN (Print): 2151-2043
Original language: English
Fundamental Studies
Source: FindIt
Source-ID: 276169282
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

High performance p-type segmented leg of misfit-layered cobaltite and half-Heusler alloy

In this study, a segmented p-type leg of doped misfit-layered cobaltite Ca_{2.8}Ag_{0.15}Co_{4}O_{9+δ} and half-Heusler Ti_{0.3}Zr_{0.35}Hf_{0.35}CoSb_{0.8}Sn_{0.2} alloy was fabricated and characterized. The thermoelectric properties of single components, segmented leg, and the electrical contact resistance of the joint part were measured as a function of temperature. The output power generation characteristics of segmented legs were characterized in air under various temperature gradients, DT, with the hot side temperature up to 1153 K. At DT ≈756 K, the maximum conversion efficiency reached a value of ~5%, which is about 65% of that expected from the materials without parasitic losses. The long-term stability investigation for two weeks at the hot and cold side temperatures of 1153/397 K shows that the segmented leg has good durability as a result of stable and low electrical resistance contacts. 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, North Carolina State University , California Institute of Technology, Johannes Gutenberg University
High performing SOFC via multilayer tape casting?

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Hauch, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
EFCF_poster_cbir_2012_06_22_hauc_edit_FINAL.pdf

Relations
Activities:
European Fuel Cell Forum 2012
Publication: Research - peer-review › Poster – Annual report year: 2015

High Temperature Electrolysis
High temperature electrolysis of carbon dioxide, or co-electrolysis of carbon dioxide and steam, has a great potential for carbon dioxide utilisation. A solid oxide electrolysis cell (SOEC), operating between 500 and 900 °C, is used to reduce carbon dioxide to carbon monoxide. If steam is also input to the cell then hydrogen is produced giving syngas. This syngas can then be further reacted to form hydrocarbon fuels and chemicals. Operating at high temperature gives much higher efficiencies than can be achieved with low temperature electrolysis. Current state of the art SOECs utilise a dense electrolyte, commonly yttria-stabilised-zirconia (YSZ), with porous fuel and oxygen side electrodes. The electrodes must be both electron and oxide ion conducting, and maximising the active surface area is essential for efficient operation. For the fuel electrode a cermet of nickel and YSZ is often used, whereas a lanthanum strontium manganite - YSZ mix is utilised for the oxygen electrode. Long term durability and performance are key for commercialisation of SOEC technology. To date, experimental tests of 1000 h on electrolysis stacks operated at low current density have shown little or no degradation when inlet gas cleaning is employed; however, operation at higher current density leads to cell degradation, which still needs to be overcome. Advances in materials and morphology are needed to further decrease cell degradation.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, University of Sheffield
Authors: Elder, R. (Ekstern), Cumming, D. (Ekstern), Mogensen, M. B. (Intern)
Number of pages: 27
Pages: 183-209
Publication date: 2015

Host publication information
Title of host publication: Carbon Dioxide Utilisation : Closing the Carbon Cycle
Publisher: Elsevier Science
Editors: Styring, P., Quadrelli, E. A., Armstrong, K.
ISBN (Print): 978-0-444-62746-9
Main Research Area: Technical/natural sciences
DOIs:
10.1016/b978-0-444-62746-9.00011-6
Source: FindIt
Source-ID: 2289319874
Publication: Research - peer-review › Book chapter – Annual report year: 2015

High-temperature stability of thermoelectric Ca₃Co₄O₉ thin films
An enhanced thermal stability in thermoelectric Ca₃Co₄O₉ thin films up to 550 °C in an oxygen rich environment was demonstrated by high-temperature electrical and X-ray diffraction measurements. In contrast to generally performed
heating in helium gas, it is shown that an oxygen/helium mixture provides sufficient thermal contact, while preventing the previously disregarded formation of oxygen vacancies. Combining thermal cycling with electrical measurements proves to be a powerful tool to study the real intrinsic thermoelectric behaviour of oxide thin films at elevated temperatures. © 2015 AIP Publishing LLC.
Hybrid direct carbon fuel cell anode processes investigated using a 3-electrode half-cell setup

A 3-electrode half-cell setup consisting of a yttria-stabilized zirconia (YSZ) electrolyte support was employed to investigate the chemical and electrochemical processes occurring in the vicinity of a model hybrid direct carbon fuel cell (HDCFC) anode (Ni-YSZ) in contact with a molten carbon-alkali carbonate slurry. Electrochemical testing, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), with and without the Ni-YSZ layer highlighted the promotional effect of the Ni-YSZ anode layer, and revealed the contributions of Ni/NiO, and potentially K/K2O, redox couple(s). Treated anthracite and bituminous coals, as well as carbon black, were tested, revealing similar open circuit potential and activation energies in mixed 96-4vol% N2-CO2 and 50-50vol% CO-CO2 environments between 700 and 800°C. Bituminous coal showed the highest activity, likely associated to a high O/C ratio and hydrogen content. Based on acquired data, a reaction scheme was proposed for processes at the working electrode, including the role of bubble formation in the vicinity of the electrochemically active solid/molten medium interface.
Hybrid Direct Carbon Fuel Cell Performance with Anode Current Collector Material

The influence of the current collector on the performance of a hybrid direct carbon fuel cell (HDCFC), consisting of solid oxide fuel cell (SOFC) with a molten carbonate-carbon slurry in contact with the anode, has been investigated using current-voltage curves. Four different anode current collectors were studied: Au, Ni, Ag, and Pt. It was shown that the performance of the direct carbon fuel cell (DCFC) is dependent on the current collector materials, Ni and Pt giving the best performance, due to their catalytic activity. Gold is suggested to be the best material as an inert current collector, due to its
low catalytic activity.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Fundamental Electrochemistry  
**Authors:** Deleebeeck, L. (Intern), Kammer Hansen, K. (Intern)  
**Number of pages:** 6  
**Publication date:** 2015  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Journal of Fuel Cell Science and Technology  
**Volume:** 12  
**Issue number:** 6  
**Article number:** 064501  
**ISSN (Print):** 1550-624X  
**Ratings:**  
  BFI (2018): BFI-level 1  
  BFI (2017): BFI-level 1  
  BFI (2016): BFI-level 1  
  Scopus rating (2016): SJR 0.226 SNIP 0.437 CiteScore 0.74  
  BFI (2015): BFI-level 1  
  Scopus rating (2015): SJR 0.222 SNIP 0.394 CiteScore 0.52  
  Web of Science (2015): Indexed yes  
  BFI (2014): BFI-level 1  
  Scopus rating (2014): SJR 0.277 SNIP 0.386 CiteScore 0.66  
  BFI (2013): BFI-level 1  
  Scopus rating (2013): SJR 0.28 SNIP 0.422 CiteScore 0.64  
  ISI indexed (2013): ISI indexed yes  
  BFI (2012): BFI-level 1  
  Scopus rating (2012): SJR 0.318 SNIP 0.388 CiteScore 0.68  
  ISI indexed (2012): ISI indexed yes  
  BFI (2011): BFI-level 1  
  Scopus rating (2011): SJR 0.369 SNIP 0.437 CiteScore 0.75  
  ISI indexed (2011): ISI indexed yes  
  BFI (2010): BFI-level 1  
  Scopus rating (2010): SJR 0.422 SNIP 0.616  
  Web of Science (2010): Indexed yes  
  BFI (2009): BFI-level 1  
  Scopus rating (2009): SJR 0.715 SNIP 0.83  
  BFI (2008): BFI-level 1  
  Scopus rating (2008): SJR 0.628 SNIP 0.859  
  Scopus rating (2007): SJR 0.559 SNIP 0.634  
  Scopus rating (2006): SJR 0.436 SNIP 0.483  
  Scopus rating (2005): SJR 0.216 SNIP 0.296  
**Original language:** English  
**DOIs:**  
10.1115/1.4032260  
**Source:** FindIt  
**Source-ID:** 2290094437  
**Publication:** Research - peer-review › Journal article – Annual report year: 2016

**Hybrid TEG-heat exchanger module for electrical power production**

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Electrofunctional materials  
**Authors:** Sarhadi, A. (Intern), Bjørk, R. (Intern), Nielsen, K. K. (Intern), Pryds, N. (Intern)  
**Number of pages:** 1
Hydrogen Energy by Means of Proton Conductors

If we dare to take serious what we know today about climate issues the challenges to our energy systems are immense. If we really choose - also in practice - to phase out the fossil fuels major changes to the way we handle energy are required. The renewable energy resources are by far sufficient, but matching supply and demand in time as well as in form calls for new engineering solutions. Hydrogen as energy carrier and energy storage medium has often been mentioned as an option for the future. A protons is an elementary particles, but at the same time the ion of hydrogen. When hydrogen (H2) is extracted from water (H2O) it can happen via formation of protons (hydrogen ions, H+) which must be transported away by proton conducting materials to form molecular hydrogen (H2). This process is called electrolysis and converts electrical energy into the chemical energy of a fuel. The reverse process of making electricity from a fuel takes place in a fuel cell. The talk will present different aspects of the concept of hydrogen energy and how materials science can bring this technology of the future closer to the present.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern)
Publication date: 2015
Event: Abstract from Tiltrædelsesforelæsning, Lyngby, Denmark.
Main Research Area: Technical/natural sciences

Bibliographical note
Inaugural Lecture (Professor)
Source: PublicationPreSubmission
Source-ID: 127806504
Publication: Communication › Conference abstract for conference – Annual report year: 2016

Identifying Activity Descriptors for CO2 Electro-Reduction to Methanol on Rutile (110) Surfaces

Electrocatalytic reduction of CO2 to liquid fuels using energy from renewable sources has the potential to form the basis of a carbon neutral sustainable energy system, while integrating seamlessly in the established infrastructure. Storing intermittent renewable energy in a chemical fuel is especially attractive to achieve high energy density required for transport applications. Among the metals, Cu electrocatalyst can convert CO2 to methane and ethylene in aqueous electrolytes at ambient temperature with moderate efficiency. However, a high overpotential is required for this reaction and almost no alcohols are produced. Experimental studies have shown that mixed rutile oxides (Ru/Ir/Ti) can catalyze the conversion of CO2 to alcohols3-5. However, very little is known about the reduction of CO2 to methanol on oxide electrocatalysts. Here, we present a computational study of the thermo-dynamics of the 6e- reduction of CO2 to methanol on substituted RuO2 (110) surfaces. We replace the Ru atoms in top layer with ten other transition metals, which in their +4 oxidation state have ionic radius comparable to Ru in octahedral coordination. The substituted surfaces show large variations in surface reactivity enabling us to explore the reduction of CO2 to methanol in a wide materials window. We use the computational hydrogen electrode model to calculate the potential dependent reaction free energies from density functional theory based calculations using BEEF-vdW functional and PAW method as implemented in VASP. We consider corrections for zero point energy, heat capacity, entropic contribution and other energy correction for CO2 and H2 molecule7. The simulation model employs ¼ monolayer of CO coverage as spectator species to emulate the presence of CO produced simultaneously by reduction of CO2. We show the electronic binding energies for reduction intermediates such as O, OCHO, HCOOH, and H2COOH scale linearly with that of OH on partially CO covered, reduced rutile surfaces. This scaling can be rationalized, by the fact all these adsorbates bind to the surfaces through the oxygen atoms. This enables us to describe the theoretical electrochemical potential required to drive the reaction as a function of the OH binding energy. Considering the OH binding energy as the prime descriptor, we can establish a volcano plot for this reaction (Figure 1). For surfaces binding OH very strongly e.g. Nb, removal of OH from active site is the most endergonic step. On the contrary, surfaces binding OH weakly e.g. Pd need large reducing potential to protonate HCOOH to methanol. While surfaces with Ir, Sn or Pt have optimal OH binding energy, for efficient methanol production, it is also important the HCOOH intermediate is bound sufficiently strongly to be further reduced to methanol. A third condition is to increase the overpotential for the parasitic production of hydrogen as much as possible. These parameters are also considered in order to evaluate the suitability of the substituted surfaces towards electrocatalytic production of methanol. We would like to acknowledge the Lundbeck Foundation for financial support of this work. References: 1. Lewis, N. S. & Nocera, D. G. Powering the planet: chemical challenges in solar energy utilization. Proc. Natl. Acad. Sci. U. S. A. 103,15729–35 (2006). doi: 10.1073/pnas.0603951103 2. Y. Hori. Electrochemical CO2 reduction on metal electrodes, in
Identifying systematic DFT errors in catalytic reactions

Using CO2 reduction reactions as examples, we present a widely applicable method for identifying the main source of errors in density functional theory (DFT) calculations. The method has broad applications for error correction in DFT calculations in general, as it relies on the dependence of the applied exchange–correlation functional on the reaction energies rather than on errors versus the experimental data. As a result, improved energy corrections can now be determined for both gas phase and adsorbed reaction species, particularly interesting within heterogeneous catalysis. We show that for the CO2 reduction reactions, the main source of error is associated with the C=O bonds and not the typically energy corrected OCO backbone.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Christensen, R. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 4
Pages: 4946-4949
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Catalysis Science & Technology
Volume: 5
Issue number: 11
ISSN (Print): 2044-4753
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.795 SNIP 1.288
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Identifying the Discharge Product and Reaction Pathway for a Secondary Mg/O-2 Battery

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan, DENSO International America, DENSO Corporation
Authors: Vardar, G. (Ekstern), Nelson, E. G. (Ekstern), Smith, J. G. (Ekstern), Naruse, J. (Ekstern), Hiramatsu, H. (Ekstern), Bartlett, B. M. (Ekstern), Sleightholme, A. E. S. (Ekstern), Siegel, D. J. (Intern), Monroe, C. W. (Ekstern)
Pages: 7564-7568
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry of Materials
Volume: 27
Issue number: 22
ISSN (Print): 0897-4756
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.89 SJR 4.114 SNIP 1.905
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.038 SNIP 2.102 CiteScore 9.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.603 SNIP 2.253 CiteScore 8.89
Web of Science (2014): Indexed yes
Impedance-Based Battery Management for Metal-O2 Systems

In electric vehicles, reliable estimation of the state-of-charge (SoC) is crucial to determine the remaining capacity, but the electrochemical processes in metal-O2 batteries are very different to the Li-ion batteries used today, and current SoC-estimation methods prove insufficient. In Li-O2 batteries, the capacity is highly dependent on the discharge rate, since different current densities enable different growth mechanisms of Li2O2, and an on-board calibration of the SoC is therefore needed. Such a calibration is typically performed by measuring the open-circuit voltage (OCV), but as the OCV of many metal-O2 battery does not change as a function of capacity, this method cannot be used. In this manuscript, we propose a method, based on a single-frequency electrochemical impedance measurement, to estimate the remaining capacity and assess the state-of-health of reversible metal-O2 batteries by calculating the capacitance of the positive electrode where the discharge products are formed. The results from experiments on Li-O2 batteries show that the capacitance is a good measure of the remaining capacity and that the SoC estimation can be improved significantly by the calibration.
Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries

Density functional theory (DFT) calculations have greatly contributed to the atomic level understanding of electrochemical reactions. However, in some cases, the accuracy can be prohibitively low for a detailed understanding of, e.g., reaction mechanisms. Two cases are examined here, i.e., the electrocatalytic reduction of CO2 and metal-air batteries. In theoretical studies of electrocatalytic CO2 reduction, calculated DFT-level enthalpies of reaction for CO2 reduction to various products are significantly different from experimental values[1-3]. In theoretical studies of metal-air battery reactions, systematic errors compared to experiments have also been found in calculation of enthalpies of formation for bulk metal oxide, peroxide and superoxide species[4,5]. It is here demonstrated how the errors, which depend explicitly on the choice of applied exchange-correlation functional, can be identified through first principle methods. Ensembles generated using a Bayesian error estimation functional, in this case the BEEF-vdW functional[6], are used for the error identification. The ensembles, which consist of perturbations of the main van der Waals density functional, can be generated at low computational cost. It has previously been demonstrated how these ensembles can be used to estimate the magnitude of functional dependent errors[6]. When here applied for identification of the source of functional dependent systematic errors, ensembles for different reactions are not only examined individually, but compared to determine patterns in functional dependence. The method is exemplified by ensemble comparison of reaction enthalpy to methanol and formic acid depicted in Figure 1. The functional dependence on the calculated reaction enthalpy to methanol is twice as large as that to formic acid. This suggests that the systematic error is due to carbon-oxygen double bonds, as the change in number of carbon-oxygen double bonds in the reaction to methanol is twice as compared to one for reaction to formic acid. This is subsequently confirmed by further comparisons of functional dependence and a significant source of systematic errors in DFT-level computational electrocatalytic CO2 reduction is hence identified. The new insight adds increased accuracy e.g., for reaction to formic acid, where the experimental enthalpy of reaction is 0.15 eV. Previously, this enthalpy has been calculated without and with correctional approaches to 0.39 eV and 0.30 eV, respectively[2]. Here, correcting the newly identified error in an otherwise similar approach as used previously the enthalpy of reaction is 0.13 eV. For metal-air batteries the previously observed large systematic errors are found not to be intrinsic to the metal oxide species. Errors can be significantly reduced by using metal chlorides as energy reference rather than pure metals. The mean absolute error per oxygen versus experiments for alkali metal peroxide and superoxide species will be 0.03 eV and 0.09 eV, respectively, using metal chlorides as reference, as compared to 0.47 eV and 0.17 eV using metals as reference. The presented approach for error identification is expected to be applicable to a very broad range of systems. References: [1] A. A. Peterson, F. Abild-Pedersen, F. Studt, J. Rossmeisl, and J. K. Nørskov, Energy Environ. Sci., 3, 1311 (2010) [2] F. Studt, F. Abild-Pedersen, J. B. Varley, and J. K. Nørskov, Catal. Lett., 143, 71 (2013) [3] K. Chan, C. Tsai, H. A. Hansen, and J. K. Nørskov, Chem. Cat. Chem., 6, 1899 (2014) [4] J. S. Hummelshøj, A. C. Luntz, and J. K. Nørskov, J. Chem. Phys., 138, 054703 (2013) [5] S. Kang, Y. Mo, S. P. Ong, and G. Ceder, Nano Lett., 14, 1016 (2014) [6] J. Wellendorff, K. T. Lundgaard, A. Megelhøj, V. Petzold, D. D. Landis, J. K. Nørskov, T. Bligaard, and K. W. Jacobsen, Phys. Rev. B, 85, 235149 (2012) Figure 1: Calculated enthalpies of reaction from CO2 to CH3OH (x axis) and HCOOH (y axis). Functional variations between the two are seen to correlate with slope 0.5 consistent with a systematic error on carbon-oxygen double bonds. [Figure]
Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging

Organic solar cells have great potential for upscaling due to roll-to-roll processing and a low energy payback time, making them an attractive sustainable energy source for the future. Active layers coated with water-dispersible Landfester particles enable greater control of the layer formation and easier access to the printing industry, which has reduced the use of organic solvents since the 1980s. Through ptychographic X-ray computed tomography (PXCT), we image quantitatively a roll-to-roll coated photovoltaic tandem stack consisting of one bulk heterojunction active layer and one Landfester particle active layer. We extract the layered morphology with structural and density information including the porosity present in the various layers and the silver electrode with high resolution in 3D. The Landfester particle layer is found to have an undesired morphology with negatively correlated top- and bottom interfaces, wide thickness distribution and only partial surface coverage causing electric short circuits through the layer. By top coating a polymer material onto the Landfester nanoparticles we eliminate the structural defects of the layer such as porosity and roughness, and achieve the increased performance larger than 1 V expected for a tandem cell. This study highlights that quantitative imaging of weakly scattering stacked layers of organic materials has become feasible by PXCT, and that this information cannot be obtained by other methods. In the present study, this technique specifically reveals the need to improve the coatability and layer formation of Landfester nanoparticles, thus allowing improved solar cells to be produced.
Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging

Project: Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging

Source: PublicationPreSubmission

Source-ID: 113783843

Publication: Research - peer-review › Journal article – Annual report year: 2015

Influence of Functionality on Direct Arylation of Model Systems as a Route Toward Fluorinated Copolymers via Direct Arylation Polymerization (DArP)

A screening of direct arylation conditions on a model small molecule system is carried out to develop suitable conditions for the direct arylation polymerization (DArP) of fluorinated copolymers, which are incompatible with conditions previously utilized successfully for nonfluorinated systems. The model system features a coupling between a 2-substituted thiophene and a pentafluorobenzene, where one of the partners was brominated. A substantial difference in reactivity is observed, demonstrating that the optimal functionalization for direct arylation between a thiophene-based donor and a highly fluorinated acceptor is a halogenated thiophene and an unfunctionalized fluorinated unit, which is opposite of typical cross-coupling reactions, where the acceptor is typically halogenated. The best conditions are applied to the copolymerization of 1,2,4,5-tetrafluorobenzene and 2,2'-(2,5-bis(2-hexyldecyloxy)21,4-phenylene)dithiophene. Polymers are free of β-defects and significant homocoupling. This work further underscores the attractive simplicity, relevance, and ease of DArP while reconfirming its broad compatibility with increasingly popular fluorinated copolymers.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Southern California
Authors: Livi, F. (Intern), Gobalasingham, N. S. (Ekstern), Bundgaard, E. (Intern), Thompson, B. C. (Ekstern)
Number of pages: 8
Pages: 2598-2605
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Polymer Science. Part A, Polymer Chemistry
Volume: 53
ISSN (Print): 0887-624X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.83 SJR 1.053 SNIP 0.781
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.002 SNIP 0.849 CiteScore 2.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.094 SNIP 0.942 CiteScore 3.05
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.154 SNIP 0.983 CiteScore 3.41
ISI indexed (2013): ISI indexed yes
Influence of hydroxyl content of binders on rheological properties of cerium-gadolinium oxide (CGO) screen printing inks

The influence of hydroxyl content of binders on rheological properties of screen printing inks is investigated. The actual amount of hydroxyl groups is correlated to the level of hyper-entanglement that characterizes the binders in solution. Three of the most used binders (ethyl cellulose, and two vinyl resins) were selected and characterized in solution via viscometry method. A high degree of hyper-entanglement was observed for ethyl cellulose polymers, whereas a mitigated effect characterized the two vinyl resins. Cerium-gadolinium oxides (CGO)-based inks, prepared using the selected binders, were investigated by means of rheology. The vinyl resin at higher hydroxyl content and low level of hyper-entanglement was demonstrated to impart superior printability properties.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Mixed Conductors, Topsoe Fuel Cell
Number of pages: 10
Pages: 1495–1504
Publication date: 2015
Main Research Area: Technical/natural sciences
Influence of interface reactions on the YBCO films grown by fluorine-free solution route

Fabrication of full-stacked coated conductors by all-chemical-solution routes exhibit a great potential in view of further reducing the cost and increasing the throughput for industrialization. Growth of YBa2Cu3O7−x (YBCO) superconducting films by fluorine-free metal organic deposition routes (FF-MOD) which are environmental friendly has attracted more attentions recently. In this work, comparison study was performed on the YBCO-Ag superconducting thin films deposited on two types of single crystal substrates, LaAlO3 and Ce0.9La0.9O2−y/YSZ. The structural characterization and superconducting properties studies reveal that the interface reactions between the YBCO-Ag film and the CLO cap layer play an essential role on the nucleation and growth of YBCO-Ag films from the FF solution. Weak texture caused by serious interface reactions at high growth temperature is the main explanations for the poor superconducting performance when using CLO/YSZ as substrate. Further investigation of compatibility of the buffer layer for FF-derived YBCO films is needed.

Influence of manganite powder grain size and Ag-particle coating on the magnetocaloric effect and the active magnetic regenerator performance

The magnetocaloric performance of La0.67Ca0.33MnO3 is investigated as a function of the powder grain size and also as a function of decoration of grains with highly conductive silver particulates as a coating layer. We demonstrate that the thermal and electrical conductivities can be significantly modified by the Ag-particle coating when the material is examined in sintered pellet form and we compare results with a second manganite composition La0.67Ca0.33MnO3 with significantly smaller grain size. However, we find that this microstructural engineering does not improve the performance of the active magnetic regenerator cycle using the silver decorated material in powder form. The regenerator performance is improved by the reduction of the powder grain size of the refrigerant which we attribute to improved thermal management due to increased surface to volume ratio. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
Influence of Side Chain Position on the Electrical Properties of Organic Solar Cells Based on Dithienylbenzothiadiazole-alt-phenylene Conjugated Polymers

Seven conjugated copolymers, based on dithienylbenzothiadiazole and benzene, have been synthesized with side chains placed in different position along the conjugated backbone. An additional polymer with a small modification of the investigated backbone was also included in the study. Alkoxy and alkyl side chains were considered, depending on the aromatic ring they were anchored to. Our goal was to perform an extensive study, by evaluating the possible anchoring positions of the same backbone, in order to demonstrate the huge influence of the position of side chains on a well performing polymer backbone for polymer solar cells. All the polymers were roll slot die coated under ambient conditions on flexible ITO-free plastic substrates to give inverted polymer solar cell devices with an upscaled active area of 1 cm².

The best characteristics were found for the polymer carrying alkoxy side chains on the benzene ring where power conversion efficiencies of up to 3.6% were achieved. All studied materials were prepared with an objective of low-cost starting materials, simple synthesis, and simple processing conditions which was most successful for the polymer P5. The polymer P7 containing fluorine atoms showed excellent performance under constant illumination and high temperature (exhibiting stable photovoltaic properties even after 670 h under conditions similar to ISOS-L-2 lifetime protocol). This makes P7 a good candidate for further upscaling and device optimization. The photovoltaic performance results were corroborated with full optical and morphological characterization of the conjugated polymers. We conclude that the determination of the best anchoring position for the side chains is the most rational starting point for the optimization of a polymer with a potential for large-scale fabrication of polymer solar cells.
Influence of SrF$_2$ on the Formation, Microstructure and Critical Temperature of (Bi,Pb)$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ Polycrystalline Samples

Bulk ceramic samples with Bi$_{1.72}$Pb$_{0.34}$Sr$_{1.87}$Ca$_{1.91}$Cu$_{3.13}$O$_{9.83-x}$F$_{2x}$ (0.00 ≤ x ≤ 0.51) nominal compositions were synthesized by a solid-state route using SrF$_2$ as a fluorine source. Notwithstanding the stage, at which SrF$_2$ was introduced into the precursor powders (prior to or after calcination), a significant lowering of the reaction temperature was observed. For a fixed sintering temperature, SrF$_2$ results in an enhanced grain growth. However, the lattice parameters of the Bi$_2$223 phase and its superconducting transition temperature are not significantly affected by the presence of fluorine. The beneficial effect of SrF$_2$ in terms of promoted Bi$_2$223 phase formation appears to be limited to low SrF$_2$ contents. It is believed that the observed effects are due to the fact that an increasing proportion of Sr is kept apart from the reaction for increasing SrF$_2$ level, rather than to a direct involvement of fluorine.
In Situ High Resolution Synchrotron X-Ray Powder Diffraction Studies of Lithium Batteries

Lithium ion battery technology is the heart in operating modern technology devices such as mobile phones and laptops. However, as our society is moving towards the utilization of sustainable energy sources, batteries can be foreseen to become an even more important part of the energy infrastructure. They will be used not only for transportation, but also for...
medium and short term storage as well as for frequency stabilization in intermittent grid scale energy sources such as solar and wind. Thus, the development of new cheaper and safer battery materials with high energy and power density is very important for a successful worldwide energy transition. The understanding of structural and compositional changes of bulk electrodes in batteries is undoubtedly important. However, it is often transport of electrons and ions across and through interfaces [1] (e.g., between lithiated and delithiated domains) which limits the obtainable power density and battery life time. A challenging and important task is to obtain in situ information about the formation and evolution of interfaces in an operating battery system. This work addresses these challenges and for this purpose we have developed a special microcapillary battery cell allowing diffraction information to be obtained from only the active material during battery operation [2]. High resolution synchrotron x-ray powder diffraction technique has been undertaken to obtain detailed structural and compositional information during lithiation/delithiation of commercial LiFePO4 materials [3]. We report results from the first in situ time resolved high resolution powder diffraction experiments at beamline ID22/31 at the European Synchrotron Radiation Facility, ESRF. We follow the structural changes during charge of commercial LiFePO4 based battery materials using the Rietveld method. Conscientious Rietveld analysis shows slight but continuous deviation of lattice parameters from those of the fully stoichiometric end members LiFePO4 and FePO4 indicating a subsequent variation of stoichiometry during cathode delithiation. The application of an intermittent current pulses during charge using GITT technique shows an oscillation of lattice constants that correlates with the applied current and electrochemical relaxation sequence and may indicate the existence of metastable non-stoichiometric states. References [1] R. Malik, F. Zhou, and G. Ceder, Nat. Mater., 10, 587 (2011). [2] R. E. Johnsen, and P. Norby, J. Appl. Crystallogr., 46, 1537 (2013). [3] A. K. Padhi, K. S. Nanjundaswamy, and J. B. Goodenough, J. Electrochem. Soc., 144, 1188 (1997).

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, European Synchrotron Radiation Facility
Authors: Amri, M. (Intern), Fitch, A. (Ekstern), Norby, P. (Intern)
Number of pages: 1
Pages: 646
Publication date: 2015
Conference: 227th ECS Meeting, Chicago, IL, United States, 24/05/2015 - 24/05/2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-01
Issue number: 2
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2015-01/2/646.abstract?sid=4aea538c-40a6-4054-8c40-6d91653d5ef4
Source: FindIt
Source-ID: 274863033
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

In Situ Studies of Fe4+ Stability in β-Li3Fe2(PO4)3 Cathodes for Li Ion Batteries

In commercial Fe-based batteries the Fe2+/Fe3+ oxidation states are used, however also utilizing the Fe4+ oxidation state, intercalation of up to two Li ions per Fe could be possible. In this study, we investigate whether Fe4+ can be formed and stabilized in β-Li3Fe2(PO4)3. The work includes in situ synchrotron X-ray powder diffraction studies (XRPD) during charging of β-Li3Fe2(PO4)3 up to 5.0 V vs. Li/Li+. A novel capillary-based micro battery cell for in situ XRPD has been designed for this. During charge, a plateau at 4.5 V was found and a small contraction in volume was observed, indicating some Li ion extraction. The volume change of the rhombohedral unit cell is anisotropic, with a decrease in the a parameter and an increase in the c parameter during the Li ion extraction. Unfortunately, no increased discharge capacity was observed and Mössbauer spectroscopy showed no evidence of Fe4+ formation. Oxidation of the organic electrolyte is inevitable at 4.5 V but this alone cannot explain the volume change. Instead, a reversible oxygen redox process (O2− → O−) could possibly explain and charge compensate for the reversible extraction of lithium ions from β-Li3Fe2(PO4)3.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Neutrons and X-rays for Materials Physics, Applied Electrochemistry, Fundamental Electrochemistry
Pages: A531-A537
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
In Situ Synchrotron X-Ray Diffraction Characterization of the Synthesis of Graphene Oxide and Reduced Graphene Oxide

Graphene oxide (GO) and reduced graphene oxide (rGO) synthesised from GO, has a promising future in fields ranging from electronics to energy technologies[1]. GO may be synthesized by the modified Hummer’s method[2], where a mixture of potassium permanganate and concentrated sulfuric acid forms the ground pillar for the oxidation of graphite to GO. rGO can be synthesized by a broad range of methods, with the chemical and the thermal reduction routes being very common[3]. The mechanism of GO by the modified Hummer’s method is still unknown, even though the active oxidizing species dimanganese heptoxide has been suggested as the main redox active species[4]. The mechanism of the thermal reduction of GO to rGO is also unknown. We present results from in situ synchrotron X-ray diffraction (XRD) experiments of syntheses and thermal reduction of GO. In the in situ synthesis of GO was performed by placing a mixture of permanganate and sulphuric acid in a capillary next to graphite. The synthesis was then initiated by gently pushing the fluid mixture into the powder with N2 gas. The in situ XRD of the GO synthesis showed how the oxidation reaction proceeds in three separate stages, as seen in Figure 1. The first stage was the dissolution of potassium permanganate, followed by an intercalation stage and subsequent formation of crystalline material. The GO 001 diffraction peak was observed early during the synthesis, in the second stage, and the intensity of the 001 diffraction increased during the third stage. The in situ XRD results of the thermal reduction of GO to rGO showed a dependence on the temperature ramping and addition of diamond powder. Syntheses were measured at 1, 5, 10, 20 and 50 °C/min temperature ramps. The syntheses were performed in a capillary with GO being heated by a hot air blower under constant N2 flow. Three stages were observed for the reduction process; a GO stage, an amorphous stage and a rGO stage. The change in stage was defined from the changing of the d-value of the initial 001 GO peak, see Figure 2. The initial GO diffraction pattern changed during the heating and more diffraction peaks were observed. The results showed that the nature of the rGO material depends heavily on both temperature and additives. These in situ XRD studies revealed the crystalline intermediates and final product of synthesis by a modified Hummer’s method and the diffractional change during the thermal reduction of GO. The stages observed for both syntheses illuminate how important it is to consider the experimental parameters dependent on the application; they might even have to be optimized separately. As the future use of GO and rGO is expanding and the commercialization of these products are enhanced, the syntheses mechanisms may be of increasing interest. [1] M. Segal, Nat Nano, 4 (2009) 612-614. [2] Hummer and Offeman, J. Am. Chem. Soc. (1958) 1339-1339 [3] Pei and Cheng, Carbon (2012) 3210-3228 [4] Dreyer, Park, Bielawski and Ruoff, Chem. Soc. Rev. (2010) 228-240 [Figure]
Sodium layered oxides with mixed transition metals have received significant attention as positive electrode candidates for sodium-ion batteries because of their high reversible capacity. The phase transformations of layered compounds during electrochemical reactions are a pivotal feature for understanding the relationship between layered structures and electrochemical properties. A combination of in situ diffraction and ex situ X-ray absorption spectroscopy reveals the phase transition mechanism for the ternary transition metal system (Fe–Mn–Co) with P2 stacking. In situ synchrotron X-ray diffraction using a capillary-based microbattery cell shows a structural change from P2 to O2 in P2–Na0.7Fe0.4Mn0.4Co0.2O2 at the voltage plateau above 4.1 V on desodiation. The P2 structure is restored upon subsequent sodiation. The lattice parameter c in the O2 structure decreases significantly, resulting in a volumetric contraction of the lattice toward a fully charged state. Observations on the redox behavior of each transition metal in P2–Na0.7Fe0.4Mn0.4Co0.2O2 using X-ray absorption spectroscopy indicate that all transition metals are involved in the reduction/oxidation process.
Instability of Ionic Liquid-Based Electrolytes in Li–O₂ Batteries

Ionic liquids (ILs) have been proposed as promising solvents for Li–air battery electrolytes. Here, several ILs have been investigated using differential electrochemical mass spectrometry (DEMS) to investigate the electrochemical stability in a Li–O₂ system, by means of quantitative determination of the rechargeability (OER/ORR), and thereby the Coulombic efficiency of discharge and charge. None of the IL-based electrolytes are found to behave as needed for a functional Li–O₂ battery but perform better than commonly used organic solvents. Also the extent of rechargeability/reversibility has been found to be strongly dependent on the choice of IL cation and anion as well as various impurities.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry, Chalmers University of Technology
Number of pages: 7
Pages: 18084–18090
Publication date: 2015
Main Research Area: Technical/natural sciences
Instability of supercritical porosity in highly doped ceria under reduced oxygen partial pressure

The thermomechanical behavior and microstructural evolution of low relative density (~0.40) gadolinium-doped ceria are characterized under oxidative and reducing conditions at high temperatures. The electronic defects generated in the structure by Ce4+ to Ce3+ reduction play an important role on all mass diffusion phenomena, including densification and grain growth. Thermodynamically stable porosity (supercritical porosity) is dominant for isothermal sintering treatments in air. Conversely, the facilitated diffusion of ions through the lattice in reducing conditions results in a nearly full densification.

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Integration of CO₂ air capture and solid oxide electrolysis for methane production

This work studied the production of substitute natural gas (SNG) from CO₂ captured from the atmosphere followed by co-electrolysis with H₂O in solid oxide electrolyzer cells (SOEC) and downstream catalytic methane production. Over the coming 20 years, Denmark is on a track to remove fossil fuels from all sectors of the energy system except for transportation. In the recently published Energikoncept 2035 [1], the Danish grid operator, Energinet.dk lays out a scenario based on 72% wind power and 21% biomass and waste in the electricity grid mix. In this scenario, biogas and electrolysis gasses are projected to be used for production of process heat, peak-load power generation and on the longer term to replace hydrocarbons in the most energy intensive parts of the transportation sector; especially aviation. As a prerequisite for the scenario, no biomass can be imported to enhance the supply of combustible resources. In such an energy system, technologies for production of CO₂ neutral hydrocarbons for easy storage and use in the existing infrastructure; especially in the natural gas grid; may be of great value. The studied technology fulfills those demands. The main goal of the work was to design a plant and develop a thermodynamic model of the plant operation, enabling analyses related to selection of operating parameters; analysis and optimization of internal heat recovery and integration between the main technological
concentrated CO2 source that can be used for enhanced oil recovery, in combination with biomass gasification and production, use of alternative fuels as well as on-site electricity production. In addition, the full oxy-fuel cases generate a those from a standard cryogenic plant. Both oxygen enriched air and full oxy-fuel cases allow for an increase in clinker and full oxy-fuel combustion in both pre-calciner and kiln are examined. The economic figures of merit are compared with economic point of view. Different configurations for oxygen enrichment of the tertiary air for combustion in the pre-calciner systems and the heat exchanger network. For operating costs, the electricity price had a significant impact, whereas the price of cell area of 0.23 €/cm2. The main cost drivers were identified as the capital costs of the SOEC and air capture €/Nm3 and 2.94 €/Nm3 based on an electricity price of 18.6 €/MJ, a price of process heat at 120 °C of 11.9 €/MJ and a acceptable rate of return set to the minimum of 4 %. The economic analysis resulted in SNG production prices of 1.88 €/Nm3 which is sufficient for injection into the natural gas grid. The SOEC stack power was around 700 kW, and the plant operated a tan energy efficiency of 65 % (HHV) and 58 % (LHV). An economic analysis based on guidelines from the Danish energy agency and standard methods was conducted accounting for interest rates, taxes, depreciation etc. at a minimum acceptable rate of return set to the minimum of 4 %. The economic analysis resulted in SNG production prices of 1.88 €/Nm3 and 2.94 €/Nm3 based on an electricity price of 18.6 €/MJ, a price of process heat at 120 °C of 11.9 €/MJ and a price of cell area of 0.23 €/cm2. The main cost drivers were identified as the capital costs of the SOEC and air capture systems and the heat exchanger network. For operating costs, the electricity price had a significant impact, whereas the dependency of the SNG price on the heat price was minor. The technical issues where discussed in separate chapters interspersed by chapters documenting the modelling and design process. Finally, a comprehensive discussion at the end treats the technical issues of the plant in the light of the economic analysis.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Ebbehøj, S. L. (Intern), Mogensen, M. B. (Intern), Jensen, S. H. (Intern), Riisager, A. (Intern)
Number of pages: 263
Publication date: 2015

Publication information
Place of publication: Roskilde
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-32-0
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Integration_of_CO2_air_capture_andSolid_oxide_electrolysis_for_methane_production.pdf

Relations
Projects:
Integration of CO2 air capture and solid oxide electrolysis for methane production
Publication: Research › Ph.D. thesis – Annual report year: 2016

Integration of oxygen membranes for oxygen production in cement plants
The present paper describes the integration of oxygen membranes in cement plants both from an energy, exergy and economic point of view. Different configurations for oxygen enrichment of the tertiary air for combustion in the pre-calculator and full oxy-fuel combustion in both pre-calciner and kiln are examined. The economic figures of merit are compared with those from a standard cryogenic plant. Both oxygen enriched air and full oxy-fuel cases allow for an increase in clinker production, use of alternative fuels as well as on-site electricity production. In addition, the full oxy-fuel cases generate a concentrated CO2 source that can be used for enhanced oil recovery, in combination with biomass gasification and
electrolysis for synthesis gas production, or possibly sequestered. The cases with oxygen enriched air provide very promising economic figures of merit with discounted payback periods slightly higher than one year. The full oxy-fuel cases have a discounted payback period of approximately 2.3 years assuming a CO2 selling price of 35 US$/ton. The sensitivity analysis of full oxy-fuel cases clearly shows that for the discounted payback period, the most sensitive parameters are the CO2 price and the clinker selling price.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Mixed Conductors, Department of Energy Conversion and Storage, F.L. Smidth A/S
Authors: Puig Arnavat, M. (Intern), Søgaard, M. (Intern), Hjuler, K. (Ekstern), Ahrenfeldt, J. (Intern), Henriksen, U. B. (Intern), Hendriksen, P. V. (Intern)
Pages: 852-865
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy
Volume: 91
ISSN (Print): 0360-5442
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.17 SJR 1.999 SNIP 1.798
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.276 SNIP 2.046 CiteScore 5.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.647 SNIP 2.63 CiteScore 5.7
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.54 SNIP 2.593 CiteScore 5.02
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.998 SNIP 2.25 CiteScore 4.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.609 SNIP 2.043 CiteScore 4
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.814 SNIP 2.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.729 SNIP 2.313
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.106 SNIP 1.444
Scopus rating (2007): SJR 0.913 SNIP 1.481
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.875 SNIP 1.306
Web of Science (2006): Indexed yes
Interfacial engineering of self-assembled monolayer modified semi-roll-to-roll planar heterojunction perovskite solar cells on flexible substrates

The morphologies of the perovskite (e.g. CH3NH3PbI3) layer are demonstrated to be critically important for highly efficient perovskite solar cells. This work applies 3-aminopropanoic acid as a self-assembled monolayer (C3-SAM) on a poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) hole transport layer (HTL) to modify the crystallinity and coverage of the CH3NH3PbI3 Cl-x(x) film, resulting in a much smoother perovskite surface morphology together with a PCE increase from 9.7% to 11.6%. Since all fabrication steps of these inverted structure devices are carried out under low temperature conditions (processing temperature <120 degrees C), it is possible to employ this method on flexible polymer substrates using roll-coating for the layer deposition. The roll-coated perovskite film on C3-SAM modified PEDOT:PSS presents a similar trend of improvement and results in enhanced PCE from 3.7% to 5.1%. The successful application of the facile HTL modification indicates a common strategy for SAM material design and selection for efficiency enhancement in perovskite photovoltaic devices.
Investigation of Impedance-Based Parameters in Metal-O2 Batteries for Next Generation of Battery Management Systems

The need for increasing driving range in electric vehicles (EV) has led to research in high capacity batteries beyond Li-ion. Metal-O2 batteries, like Li-O2 and Na-O2, have high theoretical energy densities and thus a possibility to increase the capacity of automotive batteries significantly compared to current Li-ion batteries.1,2 A battery management system (BMS) typically uses a combination of coulomb counting and calibration based on open circuit voltage (OCV) measurements that depend on the state of charge (SOC). Calibration is needed due to the accumulation of errors in the coulomb counting.3 Common for most metal-O2 batteries is that the chemistry is unchanged during discharge and charge (assuming no degradation). This means that the OCV does not change as function of SOC. Furthermore, constant current measurements show a flat discharge plateau in large parts of the discharge period. This has been shown for Li-O2 and Na-O2 batteries,4 and in some cases also for Mg-O2 and Al-O2 5,6. Taking the well studied Li-O2 battery as an example, the dominating process during discharge is reduction of oxygen to produce Li2O2 on top of an existing Li2O2 layer. As this process continues during the entire discharge, both OCV and discharge potential is constant until the end of discharge, where other processes become limiting, as shown in figure 1. New methods have to be developed to overcome the constant OCV and flat discharge plateau that otherwise would complicate both battery management and accurate online prediction of available capacity in metal-O2 batteries. Furthermore, the increased capacity predicted for the metal-O2 batteries will result in longer discharge periods without charging, thus increasing the need for accurate calibration of the capacity of metal-O2 batteries using impedance spectroscopy for calibration of the SOC tracking algorithm as well as gauging the degradation of the battery materials. This method can easily be implemented in an automotive BMS with only a few extra components and preliminary experiments have shown that the impedance measurements can be performed both during rest periods and under load conditions. This makes the method applicable not only for EVs but for batteries in a large range of electrical devices as the measurements can be performed when needed, thus maintaining a high level of accuracy for the SOC estimation and state of degradation. [1] Christensen, J., Albertus, P., Sánchez-Carrera, R. S., Lohmann, T., Kozinsky, B., Liedtke, R., et al. (2012). A Critical Review of Li/Air Batteries. Journal of the Electrochemical Society, 159(2), R1. doi:10.1149/2.086202jes [2] Hartmann, P. (2012). A rechargeable room-temperature sodium superoxide (Na2O2) battery. Nature Materials, 12(3), 228–232. doi:10.1038/nmat3486 [3] Ng, K. S., Moo, C.-S., Chen, Y.-P., & Hsieh, Y.-C. (2009). Enhanced coulomb counting method for estimating state-of-charge and state-of-health of lithium-ion batteries. Applied Energy, 86(9), 1506–1511. doi:10.1016/j.apenergy.2008.11.021 [4] McCloskey, B. D., Garcia, J. M., & Luntz, A. C. (2014). Chemical and Electrochemical Differences in Nonaqueous Li–O2 and Na–O2 Batteries. The Journal of Physical Chemistry Letters, 5(7), 1230–1235. doi:10.1021/jz500494s [5] Shiga, T., Hase, Y., Kato, Y., Inoue, M., & Takechi, K. (2013). A rechargeable non-aqueous Mg–O2 battery. Chemical Communications, 49(80), 9152–9154. doi:10.1039/c3cc434777 [6] Revel, R., Audichon, T., & Gonzalez, S. (2014). Non-aqueous aluminium-air battery based on ionic liquid electrolyte. Journal of Power Sources, 272(c), 415–421. doi:10.1016/j.jpowsour.2014.08.056 [Figure]
Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

The electrochemical performance and stability of the planar metal supported solid oxide fuel cells (MS-SOFC) with two different electrocatalytically active materials, namely, Ni:GDC and Ru:GDC was investigated. Ru:GDC with an ASR of 0.322 Ωcm² performed better compared to Ni:GDC with an ASR of 0.453 Ωcm² at 650oC. The performance of the Ru:GDC infiltrated MS-SOFC is the best measured so far on planar MS-SOFCs. It was observed that the stability of both the electrocatalytically active materials is relatively poor. Microstructure of the anode functional layer appeared to be dense up on the examination. Further optimization of microstructure, electrocatalyst amount and electrocatalyst integration process can improve the long-term stability in particular and electrochemical performance in general.

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Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

Even though solid oxide fuel cells (SOFCs) have a high potential with respect to efficiency and fuel flexibility they are not yet competitive in terms of cost and durability with conventional chemical energy conversion technologies. The potential cost reduction can be achieved through the development of metal supported SOFCs (MS-SOFCs) by using the cheaper support materials such as stainless steel. Furthermore, MS-SOFCs offer some advantages compared to conventional electrode and electrolyte supported SOFCs such as higher thermal conductivity, ductility in support, which are advantageous in tolerating the vibrations, transient loads, thermal and redox cycling [1-2]. The DTU MS-SOFC design based on ferritic stainless steel requires incorporation of electrocatalyst into the anode functional layer by infiltration methods [3]. Previously, the preferred electrocatalyst has been gadolinium doped ceria (GDC) with small amounts of Ni, which in the following is referred to as Ni:GDC. Recently, studies on Nb-doped SrTiO3 anode based all ceramic electrolyte supported SOFCs have shown that Ru:GDC electrocatalyst is relatively superior in terms of performance and durability than Ni:GDC [4]. In the present study, MS-SOFCs infiltrated with Ru:GDC electrocatalyst are investigated. The Ru:GDC precursor solution was infiltrated into the anode backbone and heat treated in air at different temperatures to remove the organic materials while preventing the corrosion of the metal particles. The morphology and microstructure of the infiltrated electrocatalyst layer was characterized using high-resolution electron microscopy. The electrochemical characterization involved polarization curves and electrochemical impedance spectroscopy (EIS) in the temperature range of 650-750°C. The polarization curve for Ru:GDC infiltrated MS-SOFC on single cell level (active area 16 cm2) is presented in Fig. 1. The fuel utilization corrected polarization resistance, Rp, of 0.322Ωcm2 was measured at 650°C in 20%H2O/H2. This is the lowest Rp reported for any MS-SOFC design to the knowledge of the authors. The durability was lower than expected and this could be due to the loss of percolation of the electrocatalyst. The relatively dense microstructure of the anode functional layer might have resulted in very thin electrocatalyst layer that could become non-percolating layer over the time at the operating temperature. Fig. 1: Polarization curve of Ru:GDC infiltrated MS-SOFC at 650°C with 20%H2O/H2 fuel and air as oxidant. References: [1] M.C. Tucker, J. Power Sources, 195 (2010) 4570-4582. [2] P. Blennow, J. Hjelm, T. Klemensso, S. Ramousse, A. Kromp, A. Leonide, A. Weber, J. Power Sources, 196 (2011) 7117-7125. [3] T. Klemensso, J. Nielsen, P. Blennow, A.H. Persson, T. Stegk, B.H. Christensen, S. Sonderby, J. Power Sources, 196 (2011) 9459-9466. [4] T. Ramos, S. Veitze, B. R. Sudireddy, P.S. Jørgensen, L. Theil Kuhn, P. Holtappels, Fuel Cells, 14 (2014) 1062-1065.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Imaging and Structural Analysis, Mixed Conductors
Authors: Sudireddy, B. R. (Intern), Nielsen, J. (Intern), Thydén, K. T. S. (Intern), Persson, Å. H. (Intern), Brodersen, K. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-03
Issue number: 1
Article number: 185
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2015

Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

The electrochemical performance and stability of the planar metal supported solid oxide fuel cells (MS-SOFC) with two different electrocatalytically active materials, namely, Ni:GDC and Ru:GDC were investigated. Ru:GDC with an ASR of 0.322 Ωcm2 performed better than Ni:GDC with an ASR of 0.453 Ωcm2 at 650°C. The performance of the Ru:GDC infiltrated MS-SOFC is the best measured so far on planar MS-SOFCs. It was observed that the stability of both the electrocatalytically active materials is relatively poor. Microstructure of the anode functional layer appeared to be dense up on the examination. Further optimization of microstructure, electrocatalyst amount and electrocatalyst integration process can improve the long-term stability in particular and electrochemical performance in general.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors, Technical University of Denmark
Authors: Sudireddy, B. R. (Intern), Nielsen, J. (Ekstern), Thydén, K. T. S. (Intern), Persson, Å. H. (Intern), Brodersen, K. (Intern)
Number of pages: 10
Pages: 1417-1426
Publication date: 2015
Kinetics of CO/CO₂ and H₂/H₂O reactions at Ni-based and ceria-based solid-oxide-cell electrodes

The solid oxide electrochemical cell (SOC) is an energy conversion technology that can be operated reversibly, to efficiently convert chemical fuels to electricity (fuel cell mode) as well as to store electricity as chemical fuels (electrolysis mode). The SOC fuel-electrode carries out the electrochemical reactions CO₂ + 2e⁻ → CO + O₂ and H₂O + 2e⁻ → H₂ + O₂, for which the electrocatalytic activities of different electrodes differ considerably. The relative activities in CO/CO₂ and H₂/H₂O and the nature of the differences are not well studied, even for the most common fuel-electrode material, a composite of nickel and yttria/scandia stabilized zirconia (Ni–SZ). Ni–SZ is known to be more active for H₂/H₂O than for CO/CO₂ reactions, but the reported relative activity varies widely. Here we compare AC impedance and DC current–overpotential data measured in the two gas environments for several different electrodes comprised of Ni–SZ, Gd-doped CeO₂ (CGO), and CGO nanoparticles coating Nb-doped SrTiO₃ backbones (CGOn/STN). 2D model and 3D porous electrode geometries are employed to investigate the influence of microstructure, gas diffusion and impurities present at reaction sites. Comparing model and porous Ni–SZ electrodes, the ratio of electrode polarization resistance in CO/CO₂ vs. H₂/H₂O decreases from 33 to 2. Experiments and modelling suggest that the ratio decreases due to a lower concentration of impurities blocking the three phase boundary and due to the nature of the reaction zone extension into the porous electrode thickness. Besides showing higher activity for H₂/H₂O reactions than CO/CO₂ reactions, the Ni/SZ interface is more active for oxidation than reduction. On the other hand, we find the opposite behaviour in both cases for CGOn/STN model electrodes, reporting for the first time a higher electrocatalytic activity of CGO nanoparticles for CO/CO₂ than for H₂/H₂O reactions in the absence of gas diffusion limitations. We propose that enhanced surface reduction at the CGOn/gas two phase boundary in CO/CO₂ and in cathodic polarization can explain why the highest reaction rate is obtained for CO₂ electrolysis. For all materials investigated, large differences observed between model
electrode kinetics and porous electrode kinetics are modelled and discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Fundamental Electrochemistry
Authors: Graves, C. R. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)
Pages: 75-95
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Faraday Discussions
Volume: 182
ISSN (Print): 1359-6640
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.051 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.7 SNIP 1.278 CiteScore 3.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.618 SNIP 1.12 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 0.948 CiteScore 3.24
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.893 SNIP 1.239 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.719 SNIP 1.22
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.799 SNIP 1.157
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.792 SNIP 1.293
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.898 SNIP 1.316
Scopus rating (2006): SJR 1.39 SNIP 1.148
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.32 SNIP 0.986
Scopus rating (2004): SJR 0.994 SNIP 0.885
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.029 SNIP 0.868
Scopus rating (2002): SJR 1.124 SNIP 0.847
Scopus rating (2001): SJR 1.249 SNIP 0.655
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.109 SNIP 0.806
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.925 SNIP 0.734
Kinetic Studies on Ni-YSZ Composite Electrodes

Introduction
Polarization of the Solid Oxide Cell (SOC) causes current to flow. If the fuel electrode is anodically polarized, the cell operates in fuel cell mode, oxidizing a fuel like hydrogen, carbon monoxide or hydrocarbons. In cathodic polarization the cell operates in electrolysis mode, reducing steam, carbon dioxide or both at the fuel electrode.

Independent of polarization direction, the current flowing through the electrodes of an SOC is limited by processes such as adsorption and desorption of reactants or products, diffusion through the porous electrodes, activation or charge transfer at the reaction sites gas conversion at the flow fields, and ohmic drop across the electrolyte. Since these processes occur in both electrodes and some of them with overlapping characteristic frequencies, it is particularly challenging to isolate and characterize a particular mechanism. Furthermore, when polarized, the cell heats up due to joule heating of the electrolyte but also the electrodes either heat or cool due to exothermic oxidation or endothermic reduction of gaseous reactant species. Kinetic investigation of SOC electrodes independent of the above effects thus requires a carefully chosen cell geometry, methodology and operation conditions. Experimental The investigated cells consist of porous Ni/8YSZ composite working-electrodes with an active area between 0.8 and 1 mm² and ~100 mm² counter electrodes of the same material screen-printed on a special shaped 8YSZ electrolyte pellet. The electrodes are sintered in air at 1350 °C. Details of the cell geometry are given elsewhere1. The cells were characterized by electrochemical impedance spectroscopy using a Gamry Reference 600TM potentiostat. Current/voltage characteristics were recorded at different temperatures and gas compositions using the same instrument. The tests are carried out in a single gas atmosphere with maximum flow rate of 6 L/h. Results and Discussion

Current density vs working electrode overpotential curves recorded in the temperature range 800 – 650°C in a 50/50 H₂/H₂O fuel mixture are displayed in figure 1(a). The curve at 700°C shows that for a current density of 100 mA/cm² in cathodic polarization, an overpotential of ca. 150 mV is required, compared with 100 mV in anodic polarization. This reflects asymmetry2–6 in the kinetics of hydrogen oxidation and steam reduction. By recording current density vs overpotential curves at H₂/H₂O ratios of 30/70, 50/50 and 70/30 as displayed in figure 1(b) it could be shown that in the potential window investigated herein the dependence of kinetics on H₂/H₂O ratio is not significant. At any given potential in the investigated window, and independent of operation mode, there is a slight increase in current density with increasing steam content consistent. This translates to a decreasing area specific resistance of the fuel electrode electrochemistry with pH₂O.

A power law dependency of -0.33 is reported in literature7. Outlook
In this work experimental results of kinetic investigations on state of the art solid oxide cell electrodes carried out using a novel solid oxide cell geometry, allowing, for the very first time, determination of kinetic parameters void of influences such as temperature and current starvation will be presented. The results will provide a basis for discussion of existing analytical descriptions of the current/overpotential relations of SOC electrodes.

References

Figures:
Figure 1: Current density vs overpotential curves recorded (a) in the temperature range 800- to 650°C in a 50/50 H₂/H₂O ratio and (b) at 800°C in H₂/H₂O ratios 30/70, 50/50 and 70/30. [Figure]
Kinetic Studies on Ni-YSZ Composite Electrodes

AC and DC techniques were applied to investigate the electrochemical reaction kinetics of porous composite Ni/8-mol% yttria-stabilized zirconia (Ni/8YSZ) solid oxide cell (SOC) electrodes using a novel pseudo-3-electrode cell geometry. From OCV impedance spectra an activation energy $E_a$ of 1.13 eV, prefactor $\alpha$ of $3.7 \cdot 10^5 \cdot T$, hydrogen and steam partial pressure dependencies $a$ and $b$ respectively of $-0.07$ and $0.22$ were determined. DC current density vs. overpotential curves compared with those predicted using the determined kinetic parameters. Apparent Butler-Volmer charge transfer coefficients $\alpha$ were determined from the current density vs. overpotential curves. Values ranging from 0.57 at 650°C to 0.64 at 850°C were determined from the anodic branch and 0.85 to 0.81 from the cathodic branch in the same range, with higher fitting accuracy in the anodic branch. The lower fitting accuracy of the cathodic branch and the need for different $\alpha$ values for each branch suggests that a simple BV model of the measured electrode kinetics is insufficient and/or different reaction mechanisms might be occurring in anodic vs cathodic polarization.

General information
State: Published
Organisations: Applied Electrochemistry, Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Njordze Fon, J. (Intern), Sudireddy, B. R. (Intern), Hjelm, J. (Intern), Graves, C. R. (Intern)
Number of pages: 16
Pages: 1169-1184
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 68
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
DOIs:
10.1149/06801.1169ecst
Publication: Research - peer-review › Conference article – Annual report year: 2016
Kinetic Studies on State of the Art Solid Oxide Cells – A Comparison between Hydrogen/Steam and Reformate Fuels

Electrochemical reaction kinetics at the electrodes of Solid Oxide Cells (SOCs) were investigated at 700 °C for two cells with different fuel electrode microstructures as well as on a third cell with a reduced active electrode area. Three fuel mixtures were investigated – hydrogen/steam and reformate fuels hydrogen/carbon-dioxide and hydrogen/methane/steam. It was found that the kinetics at the fuel electrode were exactly the same in both reformates. The hydrogen/steam fuel displayed slightly faster kinetics than the reformate fuels. Furthermore the gas conversion impedance in the hydrogen/steam fuel split into two processes with opposing temperature behavior in the reformate fuels. An 87.5% reduction in active electrode area diminishes the gas conversion impedance in the hydrogen/steam fuel at high fuel flow rates. In both reformates, the second and third lowest frequency processes merged into a single process as the gas conversion was reduced. The SOC with finer electrode microstructure displayed improved kinetics.
LaNi$_{1-x}$Co$_x$O$_{3-\delta}$ (x=0.4 to 0.7) cathodes for solid oxide fuel cells by infiltration

Performance of LaNi$_{1-x}$Co$_x$O$_{3-\delta}$ (LNC) (x=0.4 to 0.7) as a cathode in solid oxide fuel cell (SOFC) is evaluated. Symmetrical cathode/electrolyte/cathode cells for electrochemical testing are prepared by infiltration of yttria stabilized zirconia (YSZ) backbone with LNC solutions. It is showed that the cathode infiltrated with LaNi$_{0.5}$Co$_{0.5}$O$_{3-\delta}$ (LNC155) has the lowest polarization resistance and activation energy, 197 mΩ cm$^2$ at 600 °C and 0.91 eV, respectively. Therefore it is the most promising material of the LNC group for electrochemical applications. X-ray diffraction analysis revealed that none of the materials is single-phased after heat treatment at 800 °C as they contain residues of La$_2$O$_3$ and La$_2$NiO$_{4-\delta}$.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
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Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: I O P Conference Series: Materials Science and Engineering
Volume: 104
Article number: 012019
ISSN (Print): 1757-8981
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.39 SJR 0.187 SNIP 0.499
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.172 SNIP 0.281 CiteScore 0.22
Scopus rating (2014): SJR 0.186 SNIP 0.306 CiteScore 0.18
Scopus rating (2013): SJR 0.183 SNIP 0.256 CiteScore 0.16
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.161 SNIP 0.203 CiteScore 0.14
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.155 SNIP 0.149 CiteScore 0.1
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.151 SNIP 0.112
Original language: English
ENGINEERING,, NANOSCIENCE, MATERIALS, GD-DOPED CERIA
Electronic versions:
LaNi$_{1-x}$Co$_x$O$_{3-\delta}$.pdf
DOIs:
10.1088/1757-899X/104/1/012019
Source: FindIt
Source-ID: 2291593522
Publication: Research - peer-review › Journal article – Annual report year: 2016

Large-scale electricity storage utilizing reversible solid oxide cells combined with underground storage of CO$_2$ and CH$_4$

Electricity storage is needed on an unprecedented scale to sustain the ongoing transition of electricity generation from fossil fuels to intermittent energy sources like wind and solar power. Today pumped hydro is the only commercially viable large-scale electricity storage technology, but unfortunately it is limited to mountainous regions and therefore difficult to expand. Emerging technologies like adiabatic compressed air energy storage (ACAES) or storage using conventional power-to-gas (P2G) technology combined with underground gas storage can be more widely deployed, but unfortunately for long-term to seasonal periods these technologies are either very expensive or provide a very low round-trip efficiency. Here we describe a novel storage method combining recent advances in reversible solid oxide electrochemical cells with sub-surface storage of CO$_2$ and CH$_4$, thereby enabling large-scale electricity storage with a round-trip efficiency exceeding 70% and an estimated storage cost around 3 b kW$^{-1}$ h$^{-1}$, i.e., comparable to pumped hydro and much better than previously proposed technologies.

General information
State: Published
Lifetime of organic photovoltaics: Linking outdoor and indoor tests

A comprehensive outdoor study of polymer solar cells and modules for duration of one year was conducted. Different sample geometries and encapsulations were employed in order to study the spread in the lifetimes. The study is a complimentary report to previous work that focused on indoor ageing tests. Comparison of the indoor and outdoor lifetimes was performed by means of the o-diagram, which constitutes the initial steps towards establishing a method for predicting the lifetime of an organic photovoltaic device under real operational conditions based on a selection of accelerated indoor tests. Acceleration factors were determined using the ISOS-protocols, which enabled reproducible data acquisition between different laboratories and operators within the OPV community. A semi-automatic filtering method was employed.
for processing data acquired in outdoor tests. It was found that the lifetime of the samples tested under outdoor conditions was somewhere between the lifetimes of samples measured in accelerated indoor test conditions of damp heat and light soaking (ISOS-D-3 and ISOS-L-2) and in moderate indoor test conditions (shelf life and high temperature storage). The presented results reveal that while the accelerated ageing studies reveal days and weeks of lifetime for the studied samples, in outdoor real operational conditions the samples demonstrate stability up to months and seasons.
Life Time Performance Characterization of Solid Oxide Electrolysis Cells for Hydrogen Production

Solid oxide electrolysis cells (SOECs) offer a promising technological solution for efficient energy conversion and production of hydrogen or syngas. The commercialization of the SOEC technology can be promoted if SOECs can be operated at high current density with stable performance over ~5 years. In this work, long-term durability of Ni/yttria stabilized zirconia (YSZ) supported planar SOECs was investigated at 800 oC for electrolysis of steam at different current densities from 0 to -1.25 A/cm2. The SOEC cells are able to be operated at current density up to ~1 A/cm2, with a predicted life time of 2 - 3 years (continuous operation, setting 1.5 V as the upper voltage defining "end of life"). The results provide technological input to future design of electrolysis plants for hydrogen production.

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General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Sun, X. (Intern), Chen, M. (Intern), Liu, Y. (Intern), Hendriksen, P. V. (Intern)
Pages: 3359-3368
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 68
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
Life Time Performance Characterization of Solid Oxide Electrolysis Cells for Hydrogen Production

Globally the amount of electricity generated from renewable energy sources such as wind or solar energy is increasing. To integrate high amount of fluctuating renewable energy into the existing energy grid, efficient and cost competitive conversion of electricity into other kinds of energy carriers is needed. Solid oxide electrolysis cells (SOECs) offer a promising technological solution for efficient energy conversion and production of hydrogen or syngas (mixture of H2 and CO) using excess electricity from renewable energy sources. For SOECs to become commercially interesting, performance, durability, and cost are among the most critical issues. Long-term stable performance over 5-10 years of operation is generally required. The commercialization of the SOEC technology can be further promoted if SOECs can be operated at high current density, as it helps reducing electrolyser capacity cost significantly. In this work, long-term durability of Ni/yttria stabilized zirconia (YSZ) supported planar SOECs were investigated at 800 oC for electrolysis of steam. The cells, which represent the state-of-the-art SOEC technology at Technical University of Denmark (DTU), have a Ni/YSZ support and active fuel electrode, a YSZ electrolyte, a gadolinia doped ceria (CGO) barrier layer and a LSCF/CGO (LSCF: strontium and cobalt co-doped lanthanum ferrite) composite oxygen electrode. The cells were exposed to long-term galvanostatic electrolysis tests at different current densities from 0 (i.e. under open circuit voltage, OCV) to -1.25 A/cm2. Detailed electrochemical and post-mortem characterizations were further conducted in order to clarify the cell or electrode degradation mechanisms. The cells show stable performance, with a steady-state degradation rate of up to 2 %/1000 h for electrolysis tests with current densities up to -1 A/cm2. The long-term degradation is dominated by increase in serial resistance, which can be associated to a great extent with microstructure changes in the active Ni/YSZ electrode, namely Ni loss (directly reflected by an increase in the porosity) and Ni re-distribution. Operating the cells at -1.25 A/cm2 causes severe and accelerated degradation, which is associated with both the Ni/YSZ fuel electrode and the LSCF/CGO oxygen electrode. Assuming an end-of-life cell voltage of 1.5 V, the cell life time is then predicted as a function of electrolysis current density. The current generation SOEC cells produced at DTU are able to be operated at current density up to ~-0.9 A/cm2, in order to achieve a commercialization target of 5 years lifetime (for continuous electrolysis operation of hydrogen production). The cells can be operated at even higher current density, if the hydrogen production is intermittent. The results of the current work provide valuable technological inputs to future design of electrolysis plants for hydrogen production.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Sun, X. (Intern), Chen, M. (Intern), Liu, Y. (Intern), Hendriksen, P. V. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-03
Issue number: 1
Article number: 400
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015
Lithium salts for advanced lithium batteries: Li–metal, Li–O2, and Li–S

Presently lithium hexafluorophosphate (LiPF6) is the dominant Li-salt used in commercial rechargeable lithium-ion batteries (LIBs) based on a graphite anode and a 3–4 V cathode material. While LiPF6 is not the ideal Li-salt for every important electrolyte property, it has a uniquely suitable combination of properties (temperature range, passivation, conductivity, etc.) rendering it the overall best Li-salt for LIBs. However, this may not necessarily be true for other types of Li-based batteries. Indeed, next generation batteries, for example lithium–metal (Li–metal), lithium–oxygen (Li–O2), and lithium–sulfur (Li–S), require a re-evaluation of Li-salts due to the different electrochemical and chemical reactions and conditions within such cells. This review explores the critical role Li-salts play in ensuring in these batteries viability.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Uppsala University, Oak Ridge National Laboratory, Chalmers University of Technology, ALISTORE-ERI European Research Institute
Number of pages: 18
Pages: 1905-1922
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Issue number: 8
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 10.027 SNIP 4.275 CiteScore 23.85
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.792 SNIP 4.034 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.02 SNIP 3.011 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.86 SNIP 2.594 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.743 SNIP 2.513 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.861 SNIP 2.41
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.045 SNIP 1.139
Original language: English
Electronic versions:
Lithium_salts_for_advanced_lithium_batteries.pdf
DOIs:
10.1039/C5EE01215E

Bibliographical note
This article is published Open Access as part of the RSC's Gold for Gold initiative, licensed under a Creative Commons Attribution 3.0 Unported Licence.
Location Optimization for Biomass Trigeneration System with Pit Thermal Energy Storage: the Case of the City of Petrinja

The combined production of electricity, heat and cold in biomass trigeneration power plants integrated with seasonal pit thermal energy storage ensures maximum utilization of biomass resources and at the same time reduction of variable operation costs of the system. Beside optimal size of trigeneration system, location allocation problem is additional factor which need to be taken into account. In this study, optimization of the location of biomass trigeneration power plant was considered. The system combined biomass cogeneration power plant, absorbers and the seasonal pit thermal energy storage. In order to optimise location two steps optimisation has been used. In the first step, hybrid optimisation model with Genetic Algorithm and fmicon were used while in the second step model searches for minimum cost of transportation subtracted by increased costs of distribution network investment. Moreover, four case studies were done for the city of Petrinja for which economic assessment of choosing optimal and non-optimal location was performed. Case studies have shown that significant amount of yearly spending on fuel can be avoided, if the optimal location has been chosen for the power plant location. Results of analysis shows that total yearly savings for biomass with optimal location can reach up to 4.2% compared to location with highest biomass costs.

Long Term Stability Investigation of Solid Oxide Electrolysis Cell with Infiltrated Porous YSZ Air Electrode Under High Current

The increased interest in stable and low cost electrodes for solid oxide cells (SOC) has driven the research of electrode preparation to infiltration of catalyst material into porous backbone material. The infiltration method enables a reduction of amount of catalyst material and increases its activity, due to high surface area of catalyst nano particles. Advantage of infiltration is also separate production of electrolyte backbone structure with good ionic connectivity and mechanical properties. With this study we present the results of a solid oxide cell with infiltrated porous yttria stabilised zirconia (YSZ) backbone air electrode and Ni/YSZ cermet fuel electrode. The SOC was tested at electrolysis conditions under high current (up to -1 A/cm²). The porous YSZ electrodes was infiltrated with gadolinium-doped ceria oxide (CGO), to act as a barrier layer between the catalyst and the backbone, and perovskite catalyst material. Cobalt doped lanthanum nickelate was used as the perovskite catalyst due to its excellent performance. The cell was tested in steam electrolysis for at least 2000h. This initial test indicate that a stable air electrode was formed, and that the cell performance and stability matches that of a state-of-the-art SOC.
Low Carbon Energy Supply for South East Europe
South East Europe consists of several smaller countries in terms of energy systems and thus, integrating energy systems of the whole region has significant benefits for all the countries included. However, as there are large differences between energy mixes of the countries included, careful energy planning needs to be carried out in order to satisfy energy needs of all the countries of the region. Due to the significant differences in geography and the climate of different parts of the region, many different technologies need to be introduced in order to have optimal, low-carbon energy mix. In this paper, steps toward the 100% renewable energy system (RES) for the year 2050 have been presented. Novelty in this paper, compared to the similar research already being carried out, is the sustainable use of biomass in 100% RES, as this is the only way in which biomass can be considered as carbon-neutral. Smart energy systems’ approach has been used in planning of 100% RES, which considers significant integration of the electrical, heating and gas sectors. Many technologies have been employed in the year 2050, but the major share is put on photovoltaics and wind energy, followed by geothermal, solar thermal, CHPs driven on biomass, hydro power and synthetic fuel technologies. Finally, it was shown that the 100% RES in the year 2050 is cheaper than the reference system, developed for the year 2012.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Adria Section of the Combustion Institute, University of Zagreb, Aalborg University, Macedonian Academy of Arts and Science
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Pages: 660-660
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts : 10th Conference on Sustainable Development of Energy, Water and Environment Systems
Article number: SDEWES2014.1192
Main Research Area: Technical/natural sciences
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2015

Lowering the platinum loading of high temperature polymer electrolyte membrane fuel cells with acid doped polybenzimidazole membranes
Membrane electrode assemblies (MEAs) with ultra-low Pt loading electrodes were prepared for high temperature polymer electrolyte membrane fuel cells (HT-PEMFCs) based on acid doped polybenzimidazole. With no electrode binders or ionomers, the triple phase boundary of the catalyst layer was established by the acid transfer from the acid doped membrane to the electrodes and can therefore be tailored by using catalysts with varied Pt to C ratios. With a loading of ca. 0.1 mgPt/cm² on each electrode the best performance was obtained with electrodes prepared from 10 wt.% Pt/C due to the improved Pt dispersion, extended triple phase boundary upon the acid transfer and the alleviated acid flooding of the catalytic layer. The MEA delivered a peak power density of 482 mW cm⁻² for H2/O2 and 321 mW cm⁻² for H2/air, corresponding to an overall Pt utilization of 2.5 and 1.7 kW gPt⁻¹ respectively. The durability test revealed no net voltage decay during more than 1700 h of uninterrupted operation at 200 mA cm⁻² and 160 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Fernandez, S. M. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 6
Pages: 51-56
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 293
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Low-voltage FIB/SEM Tomography for 3D Microstructure Evolution of LiFePO4/C Electrode

Li-ion batteries find widespread use in many electricity storage applications, from portable devices to electric vehicles [1-3], and LiFePO4 (LFP) is one of the most common cathodes because of its long durability and high safety [4, 5] but, since
its low ionic and electronic conduction, it is always mixed with carbon black (CB) additives to increase electronic percolation in the electrode. Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) Tomography is one of the most used techniques for the study of the three-dimensional microstructure of porous electrodes [6-8]. Imaging at low-kV has been shown to be an excellent technique for studying electron percolation in Ni-network in solid oxide fuel cells [9]. In this work we study the degradation process that occurs in a LFP/C electrode by Low-kV FIB/SEM Tomography, using the low-voltage percolation technique to identify compositional changes in the CB network in three-dimensions. FIB/SEM images of a fresh and degraded cathode are compared and LFP grains are seen to crack with cycling, resulting in the formation of secondary disconnected particles with increased ionic resistivity; CB particles are instead observed to agglomerate, reducing the electrochemically active surface area. Using low voltage imaging (1 kV) a significant fraction of the large carbon agglomerates found in the aged electrode show a higher secondary electron yield compared to the fresh CB particles at low accelerating voltage. This suggests that degradation occurs both due to morphological changes and due to amorphous-crystalline phase transitions in the carbon network, resulting in non-percolating CB agglomerates. Figure 1 shows lateral Everhart – Thornley (E-T) and in-lens detector images of fresh (a, b) and degraded cathode (c, d) collected after FIB slicing. White grains are LFP, black particles are CB additive and grey regions are pores infiltrated with silicon resin to improve phase contrast [7]. The CB network appears entirely dark in the in-lens detector image of the fresh electrode (Fig. 1b). It is possible to notice some charging effects from the insulating silicon resin. The in-lens detector image of the degraded electrode (Fig. 1d) is instead characterized by the presence of big carbon agglomerates (red rings) which are brighter because they charge as the electron beam hit them. This indicates a lower electric conductivity. 3D reconstruction of the entire network (Fig. 2) revealed that the carbon phase with lower electric conductivity accounted for approximately 25% of the volume of the total carbon in the sample. This of course affects electrode capacity since a reduced electron percolation in the CB network impedes (de)lithiation process of LFP particles. References - M. Armand, J. M. Tarascon, Nature, 451, 652-657 (2008). - B. Scrosati, J. Hassoun, and Y.K. Sun, Energy Environ. Sci., 4, 3287-3295 (2011). - J.M. Tarascon, M. Armand, Nature, 414, 359-367 (2001). - A.K. Padhi, K.S. Nanjundaswamy, and J. B. Goodenough, J. Electrochem. Soc., 144(4), 1188-1194 (1997). - Y. Wang, P. He, and H. Zhou, Energy Environ. Sci., 4, 805-817 (2010). - T. Hutzenlaub et al., Electrochemical and Solid-State Letters, 15 (3), A33-A36 (2012). - M. Ender et al, J. Electrochem. Soc., 159(7), A972-A980 (2012). - Z. Liu et al., J. Power Sources, 227, 267-274 (2013). - K. Thydén, Y.L. Liu, and J.B. Bilde-Sørensen, Solid State Ionics, 178, 1984-1989 (2008).
Lanthanum strontium manganite microelectrodes with the nominal composition of (La0.75Sr0.25)0.95MnO3 and a thickness of ca 500 nm was electrochemically characterized in situ at temperatures from 660 to 850 °C using a controlled atmosphere high temperature scanning probe microscope. Impedance spectroscopy and cyclic voltammetry were performed on electrodes with diameters of 20–100 μm in oxygen, air and nitrogen both at open circuit voltage and at anodic and cathodic polarization. In situ conductance mapping, ex situ surface analysis by time-of-flight secondary ion mass spectrometry, and scanning electron microscopy were performed to observe electrical, chemical and structural changes on the microelectrodes. © 2015 The Electrochemical Society.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Fundamental Electrochemistry
Authors: Hansen, K. V. (Intern), Norrman, K. (Intern), Jacobsen, T. (Intern), Wu, Y. (Intern), Mogensen, M. B. (Intern)
Pages: F1165-F1174
Publication date: 2015
Magnesium oxide supported thin dual phase composite oxygen permeation reactors

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Ovtar, S. (Intern), Søgaard, M. (Intern), Gurauskis, J. (Intern), Hendriksen, P. V. (Intern), Kaiser, A. (Intern)
Number of pages: 2
Publication date: 2015
Event: Abstract from 12th International Conference on Catalysis in Membrane Reactors, Szczecin, Poland.
Main Research Area: Technical/natural sciences
Electronic versions:
ICCMR12_Abstract_simov_fin
Source: PublicationPreSubmission
Source-ID: 116760877
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Magnetocaloric effect and H gradient in bulk La(Fe,Si)13Hy magnetic refrigerants obtained by HDSH

Results are reported on the preparation of bulk parts of La(Fe,Si)13Hy via the Hydrogen-Decrepitation-Sintering-Hydrogenation (HDSH) process. Net shape parts for application in room-temperature magnetic refrigeration have been produced in only 8 h of heat treatment which is considerably faster than the conventional ingot homogenization heat treatment of 7 days. The samples produced by HDSH showed higher amounts of hydrogen than the parts hydrogenated by the conventional method of thermal homogenization (20 h at 1423 K), milling to fine powder and subsequent hydrogenation. Hydrogenation parameters play an important role for the stability of the desired La(Fe,Si)13 phase during the process. Hydrogen desorption was seen to occur at two temperature ranges as a result of internal gradients. Dissimilar amounts of α-Fe were precipitated for different hydrogenation times. As a result, parts produced via HDSH with 2 and 4 h of hydrogenation exhibited different magnetocaloric behaviours. For a hydrogenation step of 4 h, parts with a demagnetization factor of 0.49 showed an adiabatic temperature change (ΔTad) higher than 1 K for a temperature range of 40 K with a maximum value of 1.57 K for an applied magnetic field of 1.75 T. As the duration of the hydrogenation step of the HDSH process decreased to 2 h, ΔTad was larger than 1 K for a temperature range of 24 K. However the maximum value of ΔTad at 328 K was 2.2 K, which is 37.5% larger than the maximum value for a hydrogenation period of 4 h.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Federal University of Santa Catarina
Authors: Neves Bez, H. (Intern), Eggert, B. G. (Ekstern), Lozano, J. (Ekstern), Bahl, C. R. (Intern), Barbosa Jr., J. R. (Ekstern), Teixeira, C. S. (Ekstern), Wendhausen, P. A. P. (Ekstern)
Pages: 125–128
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 386
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Magnetocaloric Energy Conversion: From Theory to Applications

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana
Authors: Kitanovski, A. (Ekstern), Tusek, J. (Intern), Tomc, U. (Ekstern), Piaznik, U. (Ekstern), Ozbolt, M. (Ekstern), Poredos, A. (Ekstern)
Number of pages: 471
Publication date: 2015

Publication information
Publisher: Springer
ISBN (Print): 978-3-319-08740-5
ISBN (Electronic): 978-3-319-08741-2
Original language: English
Series: Green Energy and Technology
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 117915444
Publication: Research - peer-review › Book – Annual report year: 2015

Magnetostriction and magnetisation in La$_{0.67}$Ca$_{0.33}$MnO$_3$ within the Bean-Rodbell framework

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. R. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the XXIV International Materials Research Congress
Publisher: MRS
Main Research Area: Technical/natural sciences
Conference: 24th International Materials Research Congress, Cancun, Mexico, 16/08/2015 - 16/08/2015
Magnetocaloric effect, Bean-Rodbell model, LCMO, Magnetostriction
Source: PublicationPreSubmission
Source-ID: 117919628
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Making Ends Meet: Flow Synthesis as the Answer to Reproducible High-Performance Conjugated Polymers on the Scale that Roll-to-Roll Processing Demands
Continuous flow methods are employed for the controlled polymerization of the roll-to-roll (R2R) compatible polymer PBDTTTz-4 including optimization and upscaling experiments. The polymerization rate and materials’ quality can be increased significantly with the continuous flow method where reaction times down to 10 min afforded PBDTTTz-4 with high molecular weight and a constant quality. The flow method enables full control of the molecular weight via tuning of the flow speed, catalyst loading, and temperature and avoids variation in materials’ quality associated with conventional batch synthesis. Upscaling from 300 mg batch synthesis to 10 g flow synthesis affords PBDTTTz-4 with a production rate of up to 120 g day$^{-1}$ for a very simple in-house build flow reactor. An average power conversion efficiency (PCE) of 3.5% is achieved on a small scale (1 cm$^2$) and an average PCE of 3.3% is achieved on a large scale (29 cm$^2$). This shows that small device efficiencies can be scaled when using full R2R processing of flexible and encapsulated carbon-based modules without the use of vacuum, indium-tin-oxide, or silver, with the best achieving a PCE of 3.8% PCE.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 7
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Materials development: general discussion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Fundamental Electrochemistry
Number of pages: 22
Pages: 307-328
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Faraday Discussions
Volume: 182
ISSN (Print): 1359-6640
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
Matrix Organization and Merit Factor Evaluation as a Method to Address the Challenge of Finding a Polymer Material for Roll Coated Polymer Solar Cells

The results presented demonstrate how the screening of 104 light-absorbing low band gap polymers for suitability in roll coated polymer solar cells can be accomplished through rational synthesis according to a matrix where 8 donor and 13 acceptor units are organized in rows and columns. Synthesis of all the polymers corresponding to all combinations of donor and acceptor units is followed by characterization of all the materials with respect to molecular weight, electrochemical energy levels, band gaps, photochemical stability, carrier mobility, and photovoltaic parameters. The photovoltaic evaluation is carried out with specific reference to scalable manufacture, which includes large area (1 cm²), stable inverted device architecture, an indium-tin-oxide-free fully printed flexible front electrode with ZnO/PEDOT: PSS (poly(3,4-ethylenedioxythiophene):polystyrene sulfonate), and a printed silver comb back electrode structure. The matrix organization enables fast identification of active layer materials according to a weighted merit factor that includes more than simply the power conversion efficiency and is used as a method to identify the lead candidates. Based on several characteristics included in the merit factor, it is found that 13 out of the 104 synthesized polymers outperformed poly(3-hexylthiophene) under the chosen processing conditions and thus can be suitable for further development.
Mechanism of formation of thermoelectric layered cobaltates by annealing CaO-CoO thin films grown by reactive sputtering

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Linköping University, Helmholtz Centre Geesthacht Centre for Materials and Coastal Research
Mechanism of Formation of the Thermoelectric Layered Cobaltate Ca₃Co₄O₉ by Annealing of CaO–CoO Thin Films

The layered cobaltate Ca₃Co₄O₉ is of interest for energy-harvesting and heat-conversion applications because of its good thermoelectric properties and the fact that the raw materials Ca and Co are nontoxic, abundantly available, and inexpensive. While single-crystalline Ca₃Co₄O₉ exhibits high Seebeck coefficient and low resistivity, its widespread use is hampered by the fact that single crystals are too small and expensive. A promising alternative approach is the growth of highly textured and/or epitaxial Ca₃Co₄O₉ thin films with correspondingly anisotropic properties. Here, we present a two-step sputtering/annealing method for the formation of highly textured virtually phase-pure Ca₃Co₄O₉ thin films by reactive cosputtering from Ca and Co targets followed by an annealing process at 730 °C under O₂-gas flow. The thermally induced phase transformation mechanism is investigated by in situ time-resolved annealing experiments using synchrotron-based 2D X-ray diffraction (XRD) as well as ex situ annealing experiments and standard lab-based XRD. By tuning the proportion of initial CaO and CoO phases during film deposition, the method enables synthesis of Ca₃Co₄O₉ thin films as well as CaxCoO2. With this method, we demonstrate production of epitaxial Ca₃Co₄O₉ thin films with in-plane electrical resistivity of 6.44 mΩ cm and a Seebeck coefficient of 118 μV K⁻¹ at 300 K.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Linköping University, Helmholtz Centre Geesthacht Centre for Materials and Coastal Research
Authors: Paul, B. (Ekstern), Schroeder, J. L. (Ekstern), Kerdsongpanya, S. (Ekstern), Van Nong, N. (Intern), Schell, N. (Ekstern), Ostach, D. (Ekstern), Lu, J. (Ekstern), Birch, J. (Ekstern), Eklund, P. (Ekstern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences

Mechanistic Pathway in the Electrochemical Reduction of CO₂ on RuO₂

RuO₂ has been reported to reduce CO₂ electrochemically to methanol at low overpotential. Herein, we have used density functional theory (DFT) to gain insight into the mechanism for CO₂ reduction on RuO₂(110). We have investigated the thermodynamic stability of various surface terminations in the electrochemical environment and found CO covered surfaces to be particularly stable, although their formation might be kinetically limited under mildly reducing conditions. We have identified the lowest free energy pathways for CO₂ reduction to formic acid (HCOOH), methanol (CH₃OH), and methane (CH₄) on partially reduced RuO₂(110) covered with 0.25 and 0.5 ML of CO*. We have found that CO₂ is reduced to formic acid, which is further reduced to methanol and methane. At 0.25 ML of CO*, the reduction of formate (OCHO*) to formic acid is the thermodynamically most difficult step and becomes exergonic at potentials below −0.43 V vs the reversible hydrogen electrode (RHE). On the other hand, at 0.5 ML of CO*, the reduction of formic acid to H₂COOH⁺ is the thermodynamically most difficult step and becomes exergonic at potentials below −0.25 V vs RHE. We have found that
CO2 reduction activity on RuO2 changes with CO coverage, which suggests that CO coverage can be used as a tool to tune the CO2 reduction activity. We have shown the mechanism for CO2 reduction on RuO2 to be different from that on Cu. On Cu, hydrocarbons are formed at high Faradaic efficiency through reduction of CO* at ~1 V overpotential, while on RuO2, methanol and formate are formed through reduction of formic acid at lower overpotentials. Using our understanding of the CO2 reduction mechanism on RuO2, we suggest reduction of formic acid on RuO2, which should lead to methanol and methane production at relatively low overpotentials.

Method and system for the purification of exhaust gas with an electrochemical cell

The present invention relates to a method for electrochemical reduction of nitrogen oxides and concomitant oxidation of soot, as well as systems useful therefor. Such methods and systems in particular are useful in the context of exhaust gas purification, in particular for diesel engines.
Methyl phosphate formation as a major degradation mode of direct methanol fuel cells with phosphoric acid based electrolytes

Phosphoric acid and phosphoric acid doped polymer membranes are widely used as electrolytes in hydrogen based fuel cells operating at elevated temperatures. Such electrolytes have been explored for direct oxidation of methanol to further increase the versatility of the systems, however, with demonstrated lifetimes of only a few days to weeks. In this work the methyl phosphate formation from the acid and methanol is identified and proposed to be a major mechanism for the cell degradation. Proton conductivity and fuel cell durability tests validate the mechanism at high methanol contents.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Paul Scherrer Institut
Authors: Aili, D. (Intern), Vassiliev, A. (Intern), Jensen, J. O. (Intern), Schmidt, T. J. (Ekstern), Li, Q. (Intern)
Number of pages: 5
Pages: 517-521
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 279
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
Modeling constrained sintering of bi-layered tubular structures

Constrained sintering of tubular bi-layered structures is being used in the development of various technologies. Densification mismatch between the layers making the tubular bi-layer can generate stresses, which may create processing defects. An analytical model is presented to describe the densification and stress developments during sintering of tubular bi-layered samples. The correspondence between linear elastic and linear viscous theories is used as a basis for derivation of the model. The developed model is first verified by finite element simulation for sintering of tubular bi-layer system. Furthermore, the model is validated using densification results from sintering of bi-layered tubular ceramic oxygen membrane based on porous MgO and Ce0.9Gd0.1O1.95-d layers. Model input parameters, such as the shrinkage kinetics and viscous parameters are obtained experimentally using optical dilatometry and thermo-mechanical analysis. Results from the analytical model are found to agree well with finite element simulations as well as measurements from sintering experiment.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Electrofunctional materials, San Diego State University
Pages: 941–950
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 35
Issue number: 3
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Modeling of Ni Diffusion Induced Austenite Formation in Ferritic Stainless Steel Interconnects

Ferritic stainless steel interconnect plates are widely used in planar solid oxide fuel cell (SOFC) or electrolysis cell (SOEC) stacks. During stack production and operation, nickel from the Ni/YSZ fuel electrode or from the Ni contact component diffuses into the IC plate, causing transformation of the ferritic phase into an austenitic phase in the interface region. This

Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.217 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.392 SNIP 1.945
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.381 SNIP 1.724
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.146 SNIP 1.645
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.22 SNIP 1.76
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.191 SNIP 1.67
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.084 SNIP 1.637
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.037 SNIP 1.747
Scopus rating (2003): SJR 1.129 SNIP 1.497
Scopus rating (2002): SJR 1.04 SNIP 1.181
Scopus rating (2001): SJR 1.238 SNIP 1.597
Scopus rating (2000): SJR 0.99 SNIP 1.182
Scopus rating (1999): SJR 1.141 SNIP 1.156
Original language: English
Constrained sintering, Oxygen membrane, Sintering, Stress, Tubular bi-layer, Stresses, Bi-layer, Oxygen membranes, Tubular structures
DOIs:
10.1016/j.jeurceramsoc.2014.10.010
Source: FindIt
Source-ID: 272730382
Publication: Research - peer-review › Journal article – Annual report year: 2014

Modeling of Ni Diffusion Induced Austenite Formation in Ferritic Stainless Steel Interconnects

Ferritic stainless steel interconnect plates are widely used in planar solid oxide fuel cell (SOFC) or electrolysis cell (SOEC) stacks. During stack production and operation, nickel from the Ni/YSZ fuel electrode or from the Ni contact component diffuses into the IC plate, causing transformation of the ferritic phase into an austenitic phase in the interface region.
is accompanied with changes in volume and in mechanical and corrosion properties of the IC plates. In this work, kinetic
modeling of the inter-diffusion between Ni and FeCr based ferritic stainless steel was conducted, using the CALPHAD
approach with the DICTRA software. The kinetics of inter-diffusion and austenite formation was explored in full detail, as
functions of layer thickness, temperature, time, and steel composition. The simulation was further validated by comparing
with experimental results. Growth of the austenite phase in commercial interconnect materials is predicted to take place
under practical stack operation conditions.

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General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Central South University
Authors: Chen, M. (Intern), Molin, S. (Intern), Zhang, L. (Ekstern), Ta, N. (Intern), Hendriksen, P. V. (Intern), Kiebach, W.
(Intern), Du, Y. (Ekstern)
Number of pages: 10
Pages: 1691-1700
Publication date: 2015
Conference: ECS Conference on Electrochemical Energy Conversion & Storage with SOFC–XIV, Glasgow, United
Kingdom, 26/07/2015 - 26/07/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 68
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
Original language: English
Electronic versions:
Modeling_of_Ni_Diffusion_postprint.pdf
DOIs:
10.1149/06801.1691ecst
Publication: Research - peer-review › Conference article – Annual report year: 2015
Modeling the Microstructural Evolution During Constrained Sintering

A numerical model able to simulate solid-state constrained sintering is presented. The model couples an existing kinetic Monte Carlo model for free sintering with a finite element model (FEM) for calculating stresses on a microstructural level. The microstructural response to the local stress as well as the FEM calculation of the stress field from the microstructural evolution is discussed. The sintering behavior of a sample constrained by a rigid substrate is simulated. The constrained sintering results in a larger number of pores near the substrate, as well as anisotropic sintering shrinkage, with significantly enhanced strain in the central upper part of the sample surface, and minimal strain at the edges near the substrate. All these features have also previously been observed experimentally.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors
Authors: Bjørk, R. (Intern), Frandsen, H. L. (Intern), Pryds, N. (Intern)
Number of pages: 6
Pages: 3490–3495
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: American Ceramic Society. Journal
Volume: 98
Issue number: 11
ISSN (Print): 0002-7820
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1 SNIP 1.369
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.017 SNIP 1.42 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.192 SNIP 1.628 CiteScore 2.78
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.168 SNIP 1.481 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.277 SNIP 1.523 CiteScore 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.961 SNIP 1.465 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.455 SNIP 1.53
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.546 SNIP 1.433
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.444 SNIP 1.454
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.265 SNIP 1.439
Web of Science (2007): Indexed yes
Modelling of thermoelectric generators for satellite application

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Aalborg University, Quick-Ohm Küpper & Co. GmbH
Authors: Rezania, A. (Ekstern), Wijesekara, W. (Ekstern), Rosendahl, L. (Ekstern), Van Nong, N. (Intern), Bjørk, R. (Intern), Katenbrink, N. (Ekstern)
Publication date: 2015

Hosting publication information
Title of hosting publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 2C.2
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015

Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2015

Modified strontium titanates: From defect chemistry to SOFC anodes

Modified strontium titanates have received much attention recently for their potential as anode material in solid oxide fuel cells (SOFC). Their inherent redox stability and superior tolerance to sulphur poisoning and coking as compared to Ni based cermet anodes could improve durability of SOFC systems dramatically. Various substitution strategies can be deployed to optimise materials properties in these strontium titanates, such as electronic conductivity, electrocatalytic activity, chemical stability and sinterability, and thus mechanical strength. Substitution strategies not only cover choice and amount of substituent, but also perovskite defect chemistry, distinguishing between A-site deficiency (A1-xBO3) and cation-stoichiometry (ABO3+δ). Literature suggests distinct differences in the materials properties between the latter two compositional approaches. After discussing the defect chemistry of modified strontium titanates, this paper reviews three different A-site deficient donor (La, Y, Nb) substituted strontium titanates for their electrical behaviour and fuel cell performance. Promising performances in both electrolyte as well as anode supported cell designs have been obtained, when using hydrogen as fuel. Performances are retained after numerous redox cycles. Long term stability in sulphur and carbon containing fuels still needs to be explored in greater detail. This journal is

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors, Ceramic Engineering & Science, University of St Andrews, Forschungs Zentrum Jülich GmbH
Authors: Verbraeken, M. (Ekstern), Ramos, T. (Intern), Agersted, K. (Ekstern), Ma, Q. (Ekstern), Savaniu, C. (Ekstern), Sudreddy, B. R. (Intern), Irvine, J. (Ekstern), Holtappels, P. (Intern), Tietz, F. (Ekstern)
Thin films solar cells based on Cu2ZnSnS4 (CZTS) as absorber layer have seen a rapid development leading to a world record of 8.8% [1]. However, other p-type semiconductors with fewer elements and reduced complexity compared to CZTS are also available, such as ternary Cu–Sn–S systems, i.e. Cu2SnS3 (CTS) [2].
Nanoconfined LiBH₄ as a Fast Lithium Ion Conductor

Designing new functional materials is crucial for the development of efficient energy storage and conversion devices such as all solid-state batteries. LiBH₄ is a promising solid electrolyte for Li-ion batteries. It displays high lithium mobility, although only above 110 °C at which a transition to a high temperature hexagonal structure occurs. Herein, it is shown that confining LiBH₄ in the pores of ordered mesoporous silica scaffolds leads to high Li⁺ conductivity (0.1 mS cm⁻¹) at room temperature. This is a surprisingly high value, especially given that the nanocomposites comprise 42 vol% of SiO₂.

Solid state ⁷Li NMR confirmed that the high conductivity can be attributed to a very high Li⁺ mobility in the solid phase at room temperature. Confinement of LiBH₄ in the pores leads also to a lower solid-solid phase transition temperature than for bulk LiBH₄. However, the high ionic mobility is associated with a fraction of the confined borohydride that shows no phase transition, and most likely located close to the interface with the SiO₂ pore walls. These results point to a new strategy to design low-temperature ion conducting solids for application in all solid-state lithium ion batteries, which could enable safe use of Li-metal anodes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Utrecht University, Radboud University Nijmegen
Number of pages: 9
Pages: 184–192
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 25
Issue number: 2
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
Nanodomain Engineered (K, Na)NbO₃ Lead-Free Piezoceramics: Enhanced Thermal and Cycling Reliabilities

The growing environmental concerns have been pushing the development of viable green alternatives for lead-based piezoceramics to be one of the priorities in functional ceramic materials. A polymorphic phase transition has been utilized to enhance piezoelectric properties of lead-free (K, Na)NbO₃-based materials, accepting the drawbacks of high temperature and cycling instabilities. Here, we present that CaZrO₃-modified (K, Na)NbO₃ piezoceramics not only possess excellent performance at ambient conditions benefiting from nanodomain engineering, but also exhibit superior stability against temperature fluctuation and electrical fatigue cycling. It was found that the piezoelectric coefficient d₃₃ is temperature independent under 4 kV/mm, which can be attributed to enhanced thermal stability of electric field engineered domain configuration; whereas the electric field induced strain exhibits excellent fatigue resistance up to 10⁷ sesquipolar cycles. These findings render the current material an unprecedented opportunity for actuator applications demanding improved thermal and cycling reliabilities.

General information
State: Published
Organisations: Department of Wind Energy, Materials science and characterization, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Tsinghua University
Authors: Yao, F. (Ekstern), Wang, K. (Ekstern), Cheng, L. (Ekstern), Zhang, X. (Intern), Zhang, W. (Intern), Zhu, F. (Ekstern), Li, J. (Ekstern)
Pages: 448–454
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: American Ceramic Society. Journal
Volume: 98
Issue number: 2
ISSN (Print): 0002-7820
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1 SNIP 1.369
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.017 SNIP 1.42 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.192 SNIP 1.628 CiteScore 2.78
Web of Science (2014): Indexed yes
Nanoparticles and nanoimaging for organic solar cells

Solar energy is one of the few energy sources with the potential to power humanity in a future scenario where fossil fuels are not attractive due to their effect on the global climate or fossil fuels have been depleted all together. Organic photovoltaics is a promising technology for solar harvesting due to its potential for scalable roll-to-roll production and low manufacturing cost. However, the technology is faced with several obstacles which have to be overcome such as low efficiency and stability. Some of the issues are related to nano structures and device morphology. This dissertation is devoted to studying organic photovoltaics on the micro to nanometer scale, in particular photoactive Landfester particles. The ultimate goal is to increase the performance of Landfester particle layers so they can become a viable alternative to photoactive layers cast from organic solvent. Transition to a water based ink would provide a production environment without toxic fumes from organic solvents and the nanoparticle structure would provide additional morphological control. The first part of the dissertation maps photodegradation in active layers cast from organic solvents. Reduction in degradation rates is quantified for mixed electron donor and acceptor material. The spatial distribution of photodegradation in an electron donor material is mapped and the degradation is found to be homogeneous at the sub-micron length scale.
The second and third part is devoted to studying the nano structures in photoactive Landfester nanoparticles. The dispersed particles are characterized by size, internal structure and crystallinity. Crystal orientation and spatial distribution of materials are quantified for cast layers of Landfester particles. A layer of particles is also investigated in a tandem solar cell and compared to other layers in the structure using Tomographic 3D mapping. The fourth part presents a projection alignment algorithm for tomographic methods. It works by estimating projection movement through iterative logic using projection distance minimization. It is tested on simulated datasets and results in decreased angular displacements and increased spatial resolution. Further development of the algorithm could therefore be used to increase spatial resolution for characterization of organic photovoltaics and computed tomography in general.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Applied Mathematics and Computer Science , Image Analysis & Computer Graphics
Authors: Pedersen, E. B. L. (Intern), Andreasen, J. W. (Intern), Aanæs, H. (Intern)
Number of pages: 171
Publication date: 2015

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Series: ECS-Ph.D
Main Research Area: Technical/natural sciences
Publication: Research › Ph.D. thesis – Annual report year: 2015

Nano scaled electro catalysts, a versatile concept for novel solid state fuel cells and electro-catalytic reactors

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Ceramic Engineering & Science
Authors: Kammer Hansen, K. (Intern), Holtappels, P. (Intern), Ramos, T. (Intern), Sudireddy, B. R. (Intern), Traulsen, M. L. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-30
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E30_DTU_Sustain_2015.pdf

Bibliographical note
Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Need for In Operando Characterization of Electrochemical Interface Features
The problems of understanding the electrode reaction kinetics and in particular the degradation of the kinetics destroying the electrode performance, is briefly described. This is followed by an analysis of information that is needed and which knowledge may be acquired by available in operando and in situ techniques. The latter is illustrated by some examples. Further, it is discussed how research may be improved by refining and combining the available methods. Finally, possible research strategies are discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Imaging and Structural Analysis
Authors: Traulsen, M. L. (Intern), Chatzichristodoulou, C. (Intern), Hansen, K. V. (Intern), Kuhn, L. T. (Intern), Holtappels, P. (Intern), Mogensen, M. B. (Intern)
Number of pages: 18
Pages: 3-20
Need for In Operando Characterization of Electrochemical Interface Features

It has proven particularly difficult to determine the electrode reaction mechanisms in high temperature solid oxide cells (SOCs) that convert gases. The literature is full of contradictory statements and apparently contradictory findings. Often the same type of electrochemical kinetics that apply to low temperature aqueous systems are assumed valid for SOCs, but in our opinion this has not been fruitful as they do not describe the experimental findings properly. Classical room temperature wet electrochemistry has experienced a huge progress in understanding of the electrode reaction mechanisms during the recent 2 decades. This progress has to a large extent been based on combination of electrochemical characterization and in situ and in operando and in situ surface analysis techniques, which so far have been less developed for high temperature electrochemistry above 300 °C.

In spite that such techniques have only recently started becoming available for SOC electrochemistry, they are strongly needed. The high temperature solid-solid and solid-gas interfaces tend to change a lot over time due to segregation of electrolyte and electrode constituents and unavoidable trace impurities on a level of few ppm. Furthermore, a porous electrode for solid-gas reactions has three phase boundaries (TPBs), where the electrolyte, the electrode and the gaseous reactants meet. The current density will be concentrated around the TPB. Also, the TPB seems particularly prone to collect trace impurities and minority components, probably because the TPB zone has many sites with higher free energy relative to the rest of the electrode and electrolyte surface. An example of the segregation is the enrichment of yttria to the yttria stabilized zirconia (YSZ – the common SOFC electrolyte) surface, which takes place during a few hours at operation temperature. Furthermore, most often a silica rich layer will form on top of the yttria enriched layer. These “interphase” (not interface) layers may grow and change over time and with changes in temperature and other test conditions. Such segregation seems to be equally pronounced for surfaces and interfaces of the popular perovskite structured metal oxide.
electrodes such as lanthanum strontium manganites or cobaltites on which a several nanometer thick skin of strontium rich oxide forms already during cell preparation and it is believed that this is changing significantly during electrode operation. However, our knowledge about the driving forces for and the kinetics of the formation of the interphases is very superficial.

Thus, there is a strong need for in operando techniques that can characterize and monitor the development of the mentioned features as function of time and changing experimental conditions with respect to electrical, structural and chemical properties at the nano-scale. Going through the various known techniques, it becomes clear that there are not sufficient in operando techniques available to make a comprehensive electrode characterization, and therefore in situ techniques are usually employed, in which at least one of the operation conditions are fulfilled, e.g. temperature but not atmosphere is matching relevant operation conditions. Finally, our analysis of already published results points out the advantage of combining several different techniques such as electrochemical impedance spectroscopy with in operando scanning probe microscopy and surface sensitive chemical analysis methods. Examples of results will be presented.
Ni/YSZ microstructure optimization for long-term stability of solid oxide electrolysis cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Mixed Conductors
Authors: Hauch, A. (Intern), Brodersen, K. (Intern), Chen, M. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Non-destructive electrochemical graphene transfer from reusable thin-film catalysts
We demonstrate an electrochemical method - which we term oxidative decoupling transfer (ODT) - for transferring chemical vapor deposited graphene from physically deposited copper catalyst layers. This copper oxidation-based transfer technique is generally applicable to copper surfaces, and is particularly suitable where the copper is adhered to a substrate such as oxidized silicon. Graphene devices produced via this technique demonstrate 30% higher mobility than similar devices produced by standard catalyst etching techniques. The transferred graphene films cover more than 94% of target substrates - up to 100 mm diameter films are demonstrated here - and exhibit a low Raman D:G peak ratio and a homogenous and continuous distribution of sheet conductance mapped by THz time-domain spectroscopy. By applying a fixed potential of -0.4 V vs. an Ag/AgCl reference electrode - significantly below the threshold for hydrogen production by electrolysis of water - we avoid the formation of hydrogen bubbles at the graphene-copper interface, preventing delamination of thin sputtered catalyst layers from their supporting substrates. We demonstrate the reuse of the same growth substrate for five growth and transfer cycles and prove that this number is limited by the evaporation of Cu during growth of graphene. This technique therefore enables the repeated use of the highest crystallinity and purity substrates without undue increase in cost. (C) 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Nanointegration, Center for Nanostructured Graphene, Department of Energy Conversion and Storage, Proton conductors, Department of Photonics Engineering, Terahertz Technologies and Biophotonics, Columbia University, AIXTRON Ltd
Authors: Pizzocchero, F. (Intern), Jessen, B. S. (Intern), Whelan, P. R. (Intern), Kostesha, N. (Intern), Lee, S. (Ekstern), Buron, J. C. D. (Intern), Petrushina, I. (Intern), Larsen, M. B. (Intern), Greenwood, P. (Ekstern), Cha, W. J. (Ekstern), Teo, K. (Ekstern), Jepsen, P. U. (Intern), Hone, J. (Ekstern), Baggild, P. (Intern), Booth, T. (Intern)
Pages: 397-405
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Carbon
Volume: 85
ISSN (Print): 0008-6223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.49 SJR 2.077 SNIP 1.666
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.042 SNIP 1.756 CiteScore 6.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.145 SNIP 2.014 CiteScore 6.62
Non-Noble Oxygen Reduction Catalysts

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Bibliographical note
Invited Plenary Talk
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
Non-Noble Oxygen Reduction Catalysts by Means of Encapsulated Iron Carbide

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 3rd Zing Hydrogen and Fuel Cells Conference, Cancun, Mexico.
Main Research Area: Technical/natural sciences

Bibliographical note
Invited oral presentation
Source: PublicationPreSubmission
Source-ID: 127806861
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

NOx Conversion of Porous LSF15−CGO10 Cell Stacks
A porous electrochemical reactor, made of La0.85Sr0.15FeO3 as electrode and Ce0.9Gd0.1O1.95 as electrolyte, was studied for the electrochemical reduction of NO with Propene. In order to enhance the effect of polarization, the reactor was impregnated with Ce0.9Gd0.1O1.95, CeO2 or Ce0.8Pr0.2O2-d nanoparticles. The HC-SCR on the cells was increased on the impregnated cells, but no electrochemical enhancement of this was observed. The applied overpotential on the impregnated cells changed the oxidation reaction of NO into NO2 which is considered an intermediate in the NO reduction to nitrogen.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Friedberg, A. Z. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 10
Pages: 111-120
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of New Materials for Electrochemical Systems
Volume: 18
Issue number: 2
ISSN (Print): 1480-2422
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.158 SNIP 0.205 CiteScore 0.36
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.22 SNIP 0.307 CiteScore 0.39
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.228 SNIP 0.331 CiteScore 0.47
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.359 SNIP 0.351 CiteScore 0.76
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.27 SNIP 0.295 CiteScore 0.56
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.307 SNIP 0.325 CiteScore 0.61
Numerical evaluation of oxide growth in metallic support microstructures of Solid Oxide Fuel Cells and its influence on mass transport

Metal-supported Solid Oxide Fuel Cells (SOFCs) are developed as a durable and cost-effective alternative to the state-of-the-art cermet SOFCs. This novel technology offers new opportunities but also new challenges. One of them is corrosion of the metallic support, which will decrease the long-term performance of the SOFCs. In order to understand the implications of the corrosion on the mass-transport through the metallic support, a corrosion model is developed that is capable of determining the change of the porous microstructure due to oxide scale growth. The model is based on high-temperature corrosion theory, and the required model parameters can be retrieved by standard corrosion weight gain measurements. The microstructure is reconstructed from X-ray computed tomography, and converted into a computational grid. The influence of the changing microstructure on the fuel cell performance is evaluated by determining an effective diffusion coefficient and the equivalent electrical area specific resistance (ASR) due to diffusion over time. It is thus possible to assess the applicability (in terms of corrosion behaviour) of potential metallic supports without costly long-term experiments. In addition to that an analytical framework is proposed, which is capable of estimating the porosity, tortuosity and the corresponding ASR based on weight gain measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Montanuniversität Leoben, ICE Strömungsforschung GmbH
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Pages: 388-399
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 297
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Numerical Simulation of a Tapered Bed AMR

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Dall'Olio, S. (Intern), Lei, T. (Intern), Engelbrecht, K. (Intern), Bahl, C. R. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Numerical Simulation of an Tapered Bed AMR
Numerical simulation of viscoelastic free-surface flows using a streamfunction/log-conformation formulation and the volume-of-fluid method

This thesis presents a new numerical algorithm for the simulation of two-dimensional multiphase viscoelastic flows. The simulation of viscoelastic flows has both a scientific importance and practical implications in polymer processing. This work has put the emphasis on the extrusion of polymeric materials, where viscoelastic effects cause dynamical instabilities, despite the very simple geometry. This thesis reviews the popular differential constitutive models derived from molecular theories of dilute polymer solutions, polymer networks, and entangled polymer melts, as well as the inelastic phenomenological models describing shear-thinning and viscoplastic (yield stress) fluids, based on the generalized Newtonian fluid model. In addition, the numerical issues related to the high Weissenberg number problem, and its remedy with the log-conformation representation, are discussed. The proposed algorithm utilizes a new streamfunction/log-conformation scheme. The drawbacks of the classical velocity-pressure decoupled method, which is by far the most popular approach, are remedied with the pure streamfunction formulation, which is derived from the pressureless vorticity-based methods. The implicit pure streamfunction formulation is formally more accurate than the velocity-pressure decoupled method, because it is immune of decoupling errors. Moreover, the absence of decoupling enhances the stability of the calculation. The governing equations (conservation laws and constitutive models) are discretized with the finite-volume method, on a Cartesian grid. Discrete curl operators are applied to the discretized momentum equations in order to obtain the matrix system of the discrete streamfunction variables. The coupling of the streamfunction/log-conformation scheme with adaptive under-relaxation and adaptive time-stepping yield a robust and efficient viscoelastic flow solver algorithm. The potential extension of the method to threedimensional simulations is also discussed in this thesis. Bi-phasic/free-surface flows are modelled with the Volume-of-Fluid (VOF) method, and the standard piecewise-linear-interface-construction technique. In addition, a new Cellwise Conservative Unsplit (CCU) advection scheme is presented. The CCU scheme updates the liquid volume fractions based on cellwise backward-tracking of the liquid volumes. The algorithm calculates non-overlapping and conforming adjacent donating regions, which ensures the boundedness and conservativeness of the liquid volume. As a result, the CCU advection scheme is overall more accurate in classical benchmark tests, than the other state-of-the-art multidimensional VOF-advection schemes. In complex flows, the convergence rate of the CCU scheme with mesh refinements is between 2 and 3. Moreover, the remaining numerical errors are mostly due to the inability of the standard piecewise linear interface to represent subgrid material topologies (i.e. high curvatures and thin material filaments), rather than the proposed CCU advection scheme. This thesis reports examples of numerical simulations of the Oldroyd-B liquid, calculated with the proposed streamfunction/log-conformation/VOF–CCU methodology, implemented in Matlab. A thorough investigation of the viscoelastic flow in the lid-driven cavity is conducted. The streamfunction/log-conformation shows secondorder accuracy and numerical stability at very large time-step increments, which demonstrates the robustness of the scheme. The numerical results at moderate Weissenberg numbers are in good agreement with the literature. Moreover, the enhancement of numerical stability, with the streamfunction/log-conformation scheme, makes it possible to simulate elastic instabilities at high Weissenberg numbers. Quasi-periodic elastic instabilities at the upstream corner appear to be a mechanism that dissipates the stored elastic energy. The simulations of viscoelastic flows in the planar 4:1 contraction are also in good agreement with data in the literature. Finally, preliminary simulations of extrudate swelling show that the fracture melt extrusion defect could be caused by instabilities in the stress layer at the surface of the die, triggered at moderate Weissenberg numbers.
On the Defect Chemistry, Electrical Properties and Electrochemical Performances As Solid Oxide Fuel Cell Cathode Materials of New La-(Sr/Vac)-Co-Ti-O Perovskites

Perovskite-type oxides are well known materials that have been proposed as electrodes and electrolytes for solid oxide fuel cells (SOFCs). The structure, which is referred to the ABO3 stoichiometry, can accommodate many different transition metal ions in the B-site; its electronic conductivity will vary depending upon the nature and the oxidation state of these ions. On the other hand, the creation of anion vacancies or aliovalent substitution in the A position will affect to oxide ion conductivity. A proper combination of B cations and doping or vacancy creation in A-site may provide new materials with valuable properties for SOFCs. We have analysed the effect of La3+ by Sr2+ substitution and vacancies creation in several double perovskites, La2MTiO6 (M = Co, Ni, Cu). Defect chemistry and electrical behavior have been investigated in order to unveil the nature of charge carriers. Electrochemical performances have been assessed through polarization resistance measurements. In this communication we present the results regarding La2SrTiO6 perovskites. La/Sr substitution in La2-xSrxCoTiO6-δ produces Co2+ to Co3+ oxidation while vacancies in La2-xCoTiO6-δ yield Co2+ oxidation for low A-vacancy concentration. Interestingly, oxygen vacancies are predominant for higher A-vacancies concentration. These oxygen vacancies seem to be associated to La vacancies likely inhibiting oxide ion mobility. Accordingly to operating defect chemistry the electrical behavior of the La2-xSrxCoTiO6 system in a wide pO2 range is dominated by p-type electronic conduction mechanism while for La2-xCoTiO6-δ the p-type behavior is only observed at high pO2 and changes to n-type at low pO2. The contribution of oxide ion conductivity could not be unveiled due to the larger contribution of electronic component to total conductivity in the pO2 range analyzed. The preliminary evaluation of the electrodes performance reveals polarization resistances in the 0.6-0.9 Ωcm² range at 1073 K in oxygen for La2-xSrxCoTiO6-δ, which is fairly similar to the values obtained for LSM-based cathodes. However much higher polarization resistances are found for the La2-xCoTiO6-δ with values between 2.6-9.6 Ωcm² in air at 1073 K. Additional electrochemical experiments to determine performances of planar (1-2 cm²) single SOFC bearing La2-xSrxCoTiO6-δ as the cathode are now in progress.

General information
State: Published
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Number of pages: 1
Pages: 215
Publication date: 2015
Conference: 227th ECS Meeting, Chicago, IL, United States, 24/05/2015 - 24/05/2015
Main Research Area: Technical/natural sciences

Optimization of Permanent Magnet Assemblies

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bjørk, R. (Intern), Smith, A. (Intern), Bahl, C. R. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Permanent Magnet, Optimization, Finite Element Method
Electronic versions:
Optimization_of_Permanent_Magnet_Assemblies.pdf
Source: PublicationPreSubmission
Source-ID: 118647454
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Optimization of Permanent Magnet Assemblies
Optimization of spark plasma sintering conditions for antimony-doped bismuth telluride

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, Fraunhofer Institute for Material and Beam Technology
Authors: Han, L. (Intern), Van Nong, N. (Intern), Le, T. H. (Intern), Pham, H. N. (Intern), Hegelund Spangsdorf, S. (Ekstern), Roch, A. (Ekstern), Stepien, L. (Ekstern), Pryds, N. (Intern)
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 8A.3
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
ITC2015_Book_of_Abstract_03.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Optimization of the Mechanical and Electrical Performance of a Thermoelectric Module
Finite element (FE) simulation of a thermoelectric (TE) module was conducted to optimize its geometrical dimensions in terms of mechanical reliability and performance. The TE module consisted of bismuth telluride, nand p-type legs. The geometrical dimensions of the module, i.e. leg length and leg cross-sectional area, were varied and the corresponding maximum thermal stress, output power and efficiency of the module was obtained. The optimal design of the module was then suggested based on minimizing the thermal stresses and maximizing the performance, i.e. power and efficiency. The optimal dimensions at a maximum von Mises stress of 75 MPa was a leg length of 2-2.5 mm, a leg width of 1.5-2 mm, which resulted in an efficiency of 7.2. Finally, the influence of solders, i.e. solder material between the leg, the interconnector and the top ceramic layer, on the induced thermal stresses and the module performance was investigated. The results revealed that transition from elastic to plastic deformation in the solder decreases the induced thermal stresses significantly. Moreover, beyond the elastic limit the stress magnitude is very much dependent on the magnitude and mechanism of the plastic deformation in the module. The present study provides a basis for unique and new optimization scheme of the TE modules in terms of endurance and performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Sarhadi, A. (Intern), Bjørk, R. (Intern), Pryds, N. (Intern)
Pages: 4465-4472
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Electronic Materials
Volume: 44
Issue number: 11
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Over 2 Years of Outdoor Operational and Storage Stability of ITO-free, Fully Roll-to-Roll Fabricated Polymer Solar Cell Modules

We report on the stability of large-area (100 cm²), low-cost, indium-tin-oxide (ITO)-free modules over two years (>17,500 h) under outdoor operational conditions in Denmark and under indoor storage condition by following ISOS-O-3 and ISOS-D-2 protocols. Irrespective of the testing regimes (storage and outdoor), all modules maintain the maximum power point (MPP) above T80 (the duration over which a solar cell retains above 80% of its initial MPP) over two years using a simple low-cost packaging barrier with a water vapor transmission rate (WVTR) of 0.04 g m⁻² day⁻¹, an oxygen transmission rate (OTR) of 0.01 cm³ m⁻² bar⁻¹ day⁻¹, and a UV cut-off at 390 nm. Unlike previous studies, localized degradation through edges and contact points in the modules are not overwhelming even after more than two years; therefore, the differences in degradation under long-term outdoor and storage conditions could be probed. The results suggest that oxygen permeation may be mainly responsible for degradation under outdoor conditions, whereas WVTR has a larger bearing...
under storage conditions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Angmo, D. (Intern), Krebs, F. C. (Intern)
Number of pages: 10
Pages: 774-783
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Technology
Volume: 3
Issue number: 7
ISSN (Print): 2194-4288
Ratings:
Web of Science (2017): Indexed yes
Scopus rating (2016): SJR 0.283 SNIP 0.13 CiteScore 0.66
Scopus rating (2015): SNIP 0.103 SJR 0.163 CiteScore 0.21
Web of Science (2015): Indexed yes
Scopus rating (2014): SNIP 0.564 SJR 1.681
Web of Science (2014): Indexed yes
ISI indexed (2013): ISI indexed no
Original language: English
Barrier materials, Energy conversion, Outdoor, Solar cells stability, Oxygen permeable membranes, Storage (materials), Tin oxides, Barrier material, Maximum power point, Operational conditions, Oxygen transmission rates, Polymer Solar Cells, Water vapor transmission rate, Solar cells
DOIs:
10.1002/ente.201500086
Source: FindIt
Source-ID: 275412672
Publication: Research - peer-review › Journal article – Annual report year: 2015

Oxygen electrodes: general discussion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Irvine, J. (Ekstern), Gorte, R. (Ekstern), Barnett, S. (Ekstern), Vohs, J. (Ekstern), Ishihara, T. (Ekstern), Birss, V. (Ekstern), Call, A. (Ekstern), Yildiz, B. (Ekstern), Hartvigsen, J. (Ekstern), Hu, L. (Ekstern), Jiang, S. P. (Ekstern), Ni, C. (Ekstern), Han, M. (Ekstern), Mogensen, M. B. (Intern)
Number of pages: 7
Pages: 511-517
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Faraday Discussions
Volume: 182
ISSN (Print): 1359-6640
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.051 CiteScore 3.54
Web of Science (2015): Indexed yes
Oxygen permeation of dense dual phase tubular membranes supported on porous magnesium oxide

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Ovtar, S. (Intern), Gurauskis, J. (Intern), Bjørnetun Haugen, A. (Intern), Hendriksen, P. V. (Intern), Kaiser, A. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Summer school on Ionic and protonic conducting ceramic membranes for green energy applications, Valencia, Spain.
Main Research Area: Technical/natural sciences
Electronic versions:
Ovtar_abstract2
Source: PublicationPreSubmission
Source-ID: 116760940
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015
Temperature-programmed desorption (TPD) with a carrier gas was used to study the oxygen sorption and desorption properties of oxidation catalysts and solid-oxide fuel cell (SOFC) cathode materials \( \text{La}_{0.85}\text{Sr}_{0.15}\text{MnO}_{3+\delta} \) (LSM) and \( \text{La}_{0.60}\text{Sr}_{0.40}\text{Fe}_{0.80}\text{Mn}_{0.20}\text{O}_{3-\delta} \) (LSFM). The powders were characterized by X-ray diffractometry, atomic force microscopy (AFM), and BET surface adsorption. Sorbed oxygen could be distinguished from oxygen originating from stoichiometry changes. The results indicated that there is one main site for oxygen sorption/desorption. The amount of sorbed oxygen was monitored over time at different temperatures. Furthermore, through data analysis it was shown that the desorption peak associated with oxygen sorption is described well by second-order desorption kinetics. This indicates that oxygen molecules dissociate upon adsorption and that the rate-determining step for the desorption reaction is a recombination of monatomic oxygen. Typical problems with re-adsorption in this kind of TPD setup were revealed to be insignificant by using simulations. Finally, different key parameters of sorption and desorption were determined, such as desorption activation energies, density of sorption sites, and adsorption and desorption reaction order.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Department of Chemistry, University of Southern Denmark
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Number of pages: 11
Pages: 1635-1645
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemPhysChem
Volume: 16
Issue number: 8
ISSN (Print): 1439-4235
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.81 SJR 1.264 SNIP 0.771
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 1.334 SNIP 0.912 CiteScore 3.21
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.362 SNIP 0.905 CiteScore 3.12
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 1.442 SNIP 0.948 CiteScore 3.22
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 1.763 SNIP 0.955 CiteScore 3.24
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 1.719 SNIP 1.05 CiteScore 3.37
  - ISI indexed (2011): ISI indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 1.872 SNIP 1.031
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 1.91 SNIP 1.12
Oxygen transport membranes for biomass gasification and cement industry

Oxygen transport membranes (OTMs) are of particular interest for their potential applications in high purity oxygen separation, biomass gasification and carbon capture and storage in cement production. Gd0.1Ce0.9O1.95-δ (GCO) is one of the interesting materials of OTMs because of its high ionic conductivity and excellent chemical stability under strong reducing conditions. However, for special applications in mildly reducing conditions (e.g. pure oxygen production and oxy-coal combustion) the oxygen flux of GCO is not sufficient because the performance is limited by the low electronic conductivity.

In this study various routes for enhancing the electronic conductivity were investigated; either via elemental substitution or via mixing doped-ceria with another material when forming the membrane layers. The increase of electronic conductivity by substitution co-doped Gd and Pr in ceria was investigated by a microelectrode assisted Hebb-Wagner polarization. The electronic conductivity of PrxGd0.1Ce0.9-xO1.95-δ (x=0-0.4) was found to be significantly enhanced relative to that of GCO at high pO2 (1×10-8- 0.21 bar), by as much as three orders of magnitude in Pr0.4Gd0.1Ce0.5O1.95-δ. The electronic conductivity of PrxGd0.1Ce0.9-xO1.95-δ increases with increasing concentration of Pr. The drastic decline of activation energy of electron hole migration (10-15 at.%) indicates a drastic decrease of hopping energy as continuous percolating “Pr-path” forms in the Face-Centred Cubic (FCC) Unit Cell. This provides a new understanding of small polaron mechanism on basis of crystal structure along with the band structure. In addition, the ionic conductivity of Pr-doped GCO is greater than that of Pr-doped ceria upon the same dopant concentration because of the higher concentration of oxygen vacancy in Pr-doped GCO. The heavily Pr-doped samples showed lower ionic conductivity relative to that of slightly Pr-doped samples. This is due to the more pronounced defect association in heavily doped ceria. The thermal expansion coefficients (TEC) of Pr-doped GCO exhibited a nonlinear feature at 500 °C and increased with increasing dopant concentration. The sudden increase of TEC is a consequence of the increase of chemical expansion coefficient (CEC), which is induced by the chemical strain due to the increase of oxygen nonstoichiometry as the partial reduction of Pr occurs at elevated temperature. The chemical expansion coefficients were between 0.065-0.08 mol-1, in line with that of Pr-doped ceria. The oxygen flux of Pr0.05Gd0.1Ce0.85O1.95-δ was enhanced relative to GCO by one order of magnitude. For a 10 μm thick Pr0.4Gd0.1Ce0.5O1.95-5-based membrane, the estimated oxygen flux of 10 Nml cm-2 min-1 (the target for commercialization of OTMs) might be achieved at 900°C under a small oxygen potential gradient.

Substitution of Ce with Zn was also considered. ZnO-containing GCO could be sintered at a relatively lower temperature (1300°C vs. 1600°C). The solubility limit of ZnO in GCO is in the range of 2-3 at.%. As compared to GCO, the p-type electronic conductivity of Zn-doped GCO under oxidizing condition was not influenced by the dopant whilst the n-type electronic conductivity under reducing conditions was suppressed. The electronic conductivity was slightly suppressed by doping ZnO. This indicates that the zinc ion may be an interstitial defect in GCO.

Also dual phase membranes were studied. A 1-mm thick dual phase composite oxygen membrane (50vol.% Al0.02Ga0.02Zn0.96O1.02-50 vol.% Gd0.1Ce0.9O1.95-δ) with catalyst on both sides was observed to sustain an oxygen flux of 0.3 Nml cm-2 min-1 under air/N2 at 900 °C. The material was observed to be chemically stable in CO2 and SO2 at high temperature. However, the oxygen surface exchange of the material was slow so that a high performance catalyst is required to ensure fast oxygen surface exchange.
Some of the promising material combinations were also prepared as thin films on top of structural supports. An asymmetric (thin dense layer on a porous support) dual phase composite membrane of 70 vol.% Gd0.1Ce0.9O1.95-δ-30 vol.% La0.6Sr0.4FeO3-δ (GCO-LSF) was fabricated by a “one step” phase-inversion tape casting. Oxygen flux measurement as well as electrical conductivity relaxation indicates that the oxygen permeation flux of the membrane without catalyst is rate limited by oxygen surface exchange. Mass polarization through the porous support is insignificant over a wide range of oxygen partial pressure gradients. A stable high flux of ca. 7.00 (STP) ml cm-2 min-1 was observed for 200 hours at 850 °C with the membrane placed between air and CO. Partial surface decomposition was observed on the permeate side exposed to CO.

Besides above described investigations on ceria based systems also perovskite type membrane materials were investigated. Asymmetric Ba0.5Sr0.5(Co0.8Fe0.2)0.97Zr0.03O3-δ (BSCFZ)-based oxygen membranes were prepared by phase-inversion tape casting. The oxygen permeation fluxes of 1-mm thick disc and asymmetric membranes were limited by bulk diffusion and oxygen surface exchange in air/N2. The membranes were not chemically stable under the large chemical potential gradients (oxygen vs. H2/H2O) because of fast degradation induced by thermodynamic decomposition. The asymmetric membrane (without catalyst) exhibited a stable flux when tested under more mild conditions (O2/N2). A flux of 11.2 Nml cm-2 min-1 at 950°C was observed over 150 hours and 7 Nml cm-2 min-1 at 850°C was measured over 300 hours in O2/N2. Segregation of barium sulphate and cobalt oxide was found on the surface of the dense membranes, which is ascribed to the reaction between sulphur-containing binder (PESF) and BSCFZ powder. Significant loss of Co, Sr and Fe and enrichment of BaSO4 was observed on the permeate side after the long term test. This is likely due to kinetic demixing driven by the oxygen partial pressure gradient across the membrane.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Meneta Advanced Shims Technology A/S
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Number of pages: 215
Publication date: 2015

Oxygen Transport Properties of Ca/W-Substituted Lanthanum Nickelate

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Hendriksen, P. V. (Intern), Ovtar, S. (Intern)
Number of pages: 1
Pages: 177
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. 20th International Conference on Solid State Ionics (SSI-20)
Main Research Area: Technical/natural sciences
Conference: 20th International Conference on Solid State Ionics, Keystone, CO, United States, 14/06/2015 - 14/06/2015
Electronic versions:
SSI20_abstract_nickelates.pdf

Bibliographical note
Poster presentation
Source: PublicationPreSubmission
Source-ID: 116953644
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2015

Patterning of high mobility electron gases at complex oxide interfaces

Oxide interfaces provide an opportunity for electronics. However, patterning of electron gases at complex oxide interfaces is challenging. In particular, patterning of complex oxides while preserving a high electron mobility remains underexplored and inhibits the study of quantum mechanical effects where extended electron mean free paths are paramount. This letter
presents an effective patterning strategy of both the amorphous-LaAlO$_3$/SrTiO$_3$ (a-LAO/STO) and modulation-doped amorphous-LaAlO$_3$/La$_{7/8}$Sr$_{1/8}$MnO$_3$/SrTiO$_3$ (a-LAO/LSM/STO) oxide interfaces. Our patterning is based on selective wet etching of amorphous-LSM (a-LSM) thin films, which acts as a hard mask during subsequent depositions. Strikingly, the patterned modulation-doped interface shows electron mobilities up to $\sim 8700$ cm$^2$/V s at 2 K, which is among the highest reported values for patterned conducting complex oxide interfaces that usually are $\sim 1000$ cm$^2$/V s at 2K. © 2015 AIP Publishing LLC.
Percolative nature of A-site disordered \( \text{La}_{0.75}\text{Ca}_{0.25-x}\text{Sr}_x\text{MnO}_3 \) manganites

Magnetic, resistive, and magnetoresistance measurements were used to investigate the percolative nature of A-site disordered \( \text{La}_{0.75}\text{Ca}_{0.25-x}\text{Sr}_x\text{MnO}_3 \) (\( x = 0, 0.10 \)) manganites. \( \text{La}_{0.75}\text{Ca}_{0.15}\text{Sr}_{0.10}\text{MnO}_3 \) has an orthorhombic structure and second order magnetic phase transition indicates the presence of two prominent downturns \( T^* \) and \( T_{\text{ferro}} \) above the Curie temperature \( T_C \) in the derivative of the inverse susceptibility measurements. These observations are in agreement with the percolation model and the results are discussed in the light of phase separation happening in small polarons present in the insulating phase. © 2015 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, UGC-DAE Consortium for Scientific Research
Authors: Venkatesh, R. (Ekstern), Yadam, S. (Ekstern), Venkateshwarlu, D. (Ekstern), Samatham, S. S. (Ekstern), Pryds, N. (Intern), Bahl, C. R. (Intern)
Pages: 74-78
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Chemistry and Physics
Volume: 168
ISSN (Print): 0254-0584
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.14 SJR 0.651 SNIP 0.902
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.708 SNIP 1.004 CiteScore 2.32
In this work, recent pressurized test results of a planar Ni-YSZ (YSZ: Yttria stabilized Zirconia) supported solid oxide cell are presented. Measurements were performed at 800°C in both fuel cell and electrolysis mode at different pressures. A comparison of the electrochemical performance of the cell at 1 and 3 bar shows a significant and equal performance gain at higher pressure in both fuel cell mode and electrolysis mode. Electrochemical impedance spectroscopy revealed that the serial resistance was not affected by the operation pressure; all the other processes that are dependent on partial pressures (oxygen, steam and hydrogen) were affected by increasing the pressure. In electrolysis mode at low current density, the performance improvement was counteracted by the increase in open circuit voltage, but it has to be borne in mind that the pressurized gas contains higher molar free energy.

Performance Characterization of Solid Oxide Cells Under High Pressure
In this work, recent pressurized test results of a planar Ni-YSZ (YSZ: Yttria stabilized Zirconia) supported solid oxide cell are presented. Measurements were performed at 800°C in both fuel cell and electrolysis mode at different pressures. A comparison of the electrochemical performance of the cell at 1 and 3 bar shows a significant and equal performance gain at higher pressure in both fuel cell mode and electrolysis mode. Electrochemical impedance spectroscopy revealed that the serial resistance was not affected by the operation pressure; all the other processes that are dependent on partial pressures (oxygen, steam and hydrogen) were affected by increasing the pressure. In electrolysis mode at low current density, the performance improvement was counteracted by the increase in open circuit voltage, but it has to be borne in mind that the pressurized gas contains higher molar free energy.
Performance Factors and Sulfur Tolerance of Metal Supported Solid Oxide Fuel Cells with Nanostructured Ni:GDC Infiltrated Anodes

Two metal supported solid oxide fuel cells (active area 16 cm$^2$) with nanostructured Ni:GDC infiltrated anodes, but different anode and support microstructures were studied in respect to sulfur tolerance at the aimed operating temperature of 650°C. The studied MS-SOFCs are based on ferretic stainless steel (FeCr) and showed excellent performance characteristics at 650°C with area specific resistances (ASR) of 0.35 Ωcm$^2$ and 0.7 Ωcm$^2$ respectively. The sulfur tolerance testing was performed by addition/removal of 2, 5, and 10 ppm H2S in hydrogen based fuel under galvanostatic operation at a current load of 0.25Acm$^{-2}$. The results were compared with literature on the sulfur tolerance of the conventional SOFC Ni/YSZ cermet anode. The comparison in terms of absolute cell resistance increase and relative anode polarization resistance increase indicate, that the nanostructured Ni:GDC MS-SOFC based anode is significantly more sulfur tolerant than the conventional Ni/YSZ cermet anode. © 2015 ECS - The Electrochemical Society
Performance Factors and Sulfur Tolerance of Metal Supported Solid Oxide Fuel Cells with Nanostructured Ni:GDC Infiltrated Anodes

In recent years, there has been a growing interest in developing metal supported solid oxide fuel cells (MS-SOFCs). MS-SOFCs are interesting as they potentially offer some advantages compared to conventional electrode and electrolyte supported SOFCs, such as low materials cost, better thermal conductivity and ductility of the support. The two later aspects improve the shock resistance and lower internal gradients within the stacks. This enables fast start-up and provides higher tolerance towards operation under transient conditions that are particularly desirable for APU applications. Today’s commercially available and relevant SOFC fuels such as natural gas and diesel etc. contain trace amounts of sulfur. Thus, tolerance towards sulfur poisoning is desirable. Ceria and gadolinium doped ceria (GDC) have been reported in the literature to have a beneficial effect on the tolerance towards sulfur poisoning. The ceria can be incorporated as a Ni:GDC cermet anode, but also via infiltration of ceria and doped ceria into the conventional Ni:YSZ cermet anode. Both approaches have been reported to improve the tolerance towards sulfur poisoning [1-3]. In the present study we report the performance and sulfur tolerance of MS-SOFCs with two different microstructures of the support and the anode functional layer (AFL). The MS-SOFCs of the present study are based on ferritic stainless steel (FeCr) with an aimed operating temperature of 650ºC. This lower operating temperature compared to electrode and electrolyte supported SOFCs (750ºC-850ºC) is expected to favor sulfur adsorption and hence increase the impact of sulfur poisoning. The AFL was infiltrated with Ni-GDC precursor solution and subsequent heat treated resulting in a nanostructured coating of the electrocatalyst. The two studied MS-SOFC single cells (active area 16 cm2) have initial area specific resistances (ASR) at 650ºC of 0.35 Ωcm2 and 0.7 Ωcm2 respectively. It was found that the porosity of the support and the AFL seems to have a pronounced effect on the resulting performance. The MS-SOFCs were subjected to technologically relevant H2S concentrations of 2, 5 and 10 ppm in hydrogen fuel, during galvanostatic operation at a current load of 0.25 Acm-2. The results are illustrated and compared with the conventional SOFC Ni:YSZ cermet anode in figure 1, where the relative increase in anode polarization resistance as a function of Ni sulfur coverage is shown. The comparison indicate the MS-SOFC anode of the present study to be more tolerant towards sulfur poisoning than the conventional Ni:YSZ cermet anode. [1] K. Sasaki et al., J. Electrochem. Soc., 153, A2023–A2029 (2006). [2] L. Zhang et al., International Journal of Hydrogen Energy, 35, 12359–12368 (2010). [3] C. Xu, P. Gansor, J. W. Zondlo, K. Sabolsky, and E. M. Sabolsky, J. Electrochem. Soc., 158, B1405–B1416 (2011). [Figure]
Phosphoric acid doped polysulfone membranes with aminopyridine pendant groups and imidazole cross-links

Udel polysulfone based membranes with 4-aminopyridine pendant groups and cross-linking imidazole units are synthesized in a simple two step reaction. The ratio of 4-aminopyridine and imidazole is varied and the materials are extensively characterized. The average phosphoric acid uptake (in 85 wt% PA) ranges between 90 wt% and 452 wt% depending on the ratio of 4-aminopyridine and imidazole and the membranes show good proton conductivity of up to 65 mS cm\(^{-1}\) at 160 °C under non-humidified conditions. The applicability of these materials as a polymer electrolyte membrane was proven by single cell tests at 130 °C. The relationships between PA uptake, chemical composition and mechanical stability are reported. Proton conductivity and mechanical properties only depend on the phosphoric acid content, which, however is a function of the chemical composition.
High temperature polymer electrolyte membrane fuel cell (HT-PEMFC), Udel polysulfone, Aminopyridine
Photochemical stability of random poly(3-hexylthiophene-co-3-cyanothiophene) and its use in roll coated ITO-free organic photovoltaics

The photochemical stability of the active layer blend for organic solar cells was explored by introducing electron withdrawing cyano groups into the backbone of poly-3-hexylthiophene (P3HT). Random copolymerization of 2-bromo-3-hexyl-5-trimethylstannylthiophene and 2-bromo-3-cyano-5-trimethylstannylthiophene enabled introduction of the cyanogroups along the polythiophene backbone. The percentage of the cyano groups was 10%. The photochemical stability of poly(3-hexylthiophene-co-3-cyanothiophene) (CN-P3HT) was shown to be significantly better than pristine P3HT and the addition of CN-P3HT to P3HT also increased the photochemical stability of the blend. The photochemical stability of bulk heterojunction mixtures of the polymers and their blends with the fullerene phenyl-C61-butyric acid methyl ester ([60]PCBM) were then studied and it was found that [60]PCBM had a significantly more stabilizing effect on P3HT than CN-P3HT and that the stabilization of the bulk heterojunction mixture was dominated by the fullerene. The mixture comprising both fullerene and CN-P3HT, however, demonstrated the highest degree of photochemical stability supporting earlier observations that the stabilizing effects are additive. Finally, the blends were explored in fully printed flexible ITO-free roll coated inverted devices (with an active area of 0.8 cm2) using two different back PEDOT: PSS electrode compositions and the operational stability of the devices was studied under ISOS-L-2 conditions. The pure P3HT:PCBM devices were found to be the most stable in operation demonstrating that photochemical stability alone is not necessarily the dominant factor for overall device stability.

General information
State: Published
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Number of pages: 9
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Photonics for Energy
Volume: 5
Issue number: 1
Article number: 057205
ISSN (Print): 1947-7988
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.8
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.28
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.41
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.9
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Original language: English

Active blend stabilization, Organic photovoltaic, Photochemical stability, Random copolymers, Roll-to-roll, Butyric acid, Conducting polymers, Copolymers, Fullerenes, Heterojunctions, Mixtures, Plastic coatings, Solar cells, Stability, Electrode
Photodegradation of odorous 2-mercaptobenzoxazole through zinc oxide/hydroxyapatite nanocomposite

In this study, ZnO/HAP nanocomposite with excellent photocatalytic activities was successfully synthesized by sol–gel method and used for degradation of 2-mercaptobenzoxazole (MBO) as model of odorous mercaptan compound in water. To optimize the performance of ZnO/HAP photocatalytic capabilities, ZnO/HAP loading (0.05–0.3 g/L), irradiation time (15–180 min), pH (3–11) and initial concentration of MBO (10–100 ppm) were investigated. At neutral pH of 7, the highest amount of the MBO (99.45 %) was degraded by ZnO/HAP nanocomposite through photocatalytic oxidation process within 2 h of irradiation time. A maximum adsorption capacity of 197.64 mg g−1 was obtained for ZnO/HAP under optimized conditions. BET results indicated that ZnO/HAP had a surface area of 182.36 m2g−1 which was much greater than pure ZnO nanoparticles (31.2 mg2g−1). TEM image demonstrated a spherical shape structure of ZnO/HAP with average particle size of 25 nm in diameter. The XRD patterns revealed the principal components of ZnO/HAP including HAP and ZnO. FTIR spectrum results supported formation ZnO and HAP by their stretching mode in composite. Comparison of photocatalytic activity of ZnO/HAP with pure ZnO and HAP nanoparticles had clearly recognized that latter is the most active photocatalyst in the degradation of MBO using UV light as source energy. The reason for greater activity of ZnO/HAP was due to its larger specific surface area (182.36 m2g−1) and high generation of active \(\text{HO}^\cdot\) and \(\text{O}_2^{- 2 \cdot}\) species.

Planar half-cell shaped precursor body

The invention relates to a half-cell shaped precursor body of either anode type or cathode type, the half-cell shaped precursor body being prepared to be free sintered to form a sintered or pre-sintered half-cell being adapted to be stacked in a solid oxide fuel cell stack. The obtained half-cell has an improved planar shape, which remains planar also after a sintering process and during temperature fluctuations.
Planning of Future Energy Systems Focusing on Exergy Destruction Minimization

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities
Authors: Dominkovic, D. F. (Intern), Pedersen, A. S. (Intern), Sveinbjörnsson, D. Þ. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-22
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E22_DTU_Sustain_2015.pdf

Bibliographical note
Poster presentation
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2015

Plasma properties during magnetron sputtering of lithium phosphorous oxynitride thin films
The nitrogen dissociation and plasma parameters during radio frequency sputtering of lithium phosphorus oxynitride thin films in nitrogen gas are investigated by mass appearance spectrometry, electrostatic probes and optical emission spectroscopy, and the results are correlated with electrochemical properties and microstructure of the films. Low pressure and moderate power are associated with lower plasma density, higher electron temperature, higher plasma potential and larger diffusion length for sputtered particles. This combination of parameters favors the presence of more atomic nitrogen, a fact that correlates with a higher ionic conductivity. Despite of lower plasma density the film grows faster at lower pressure where the higher plasma potential, translated into higher energy for impinging ions on the substrate, resulted in a compact and smooth film structure. Higher pressures showed much less nitrogen dissociation and lower ion energy with thinner films, less ionic conductivity and poor film structure with large roughness.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Electrofunctional materials, Imaging and Structural Analysis, Fundamental Electrochemistry
Authors: Christiansen, A. S. (Intern), Stamate, E. (Intern), Thydén, K. T. S. (Intern), Younesi, R. (Intern), Holtappels, P. (Intern)
Pages: 863-872
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 273
ISSN (Print): 0378-7753
Polarization induced changes in LSM thin film electrode composition were investigated by utilizing in operando Raman spectroscopy and post mortem TOF-SIMS depth profiling. Experiments were conducted on cells with 160 nm thick (La0.85Sr0.15)0.9MnO3±δ thin film electrodes in 10% O2 at 700 °C under various electrical polarizations. Raman spectra recorded during polarization showed shifts in spectral intensities that were both reversible and dependent on the applied potential. Spectral changes were assigned to changes in the LSM electronic structure that resulted from changing oxide concentrations in the near-surface region. Ex situ TOF-SIMS depth profiles were recorded through the LSM electrodes and revealed distinct compositional changes throughout the electrodes. The electrode elements and impurities separated into well-defined layers that were more stratified for stronger applied polarizations. The mechanism(s) behind this layering remain unidentified and highlight important questions about mass transfer and ion migration in conducting metal oxide materials subject to electrical polarization.
Polarization Induced Changes in LSM Thin Film Electrode Composition Observed by In Operando Raman Spectroscopy and TOF-SIMS

For decades strontium doped lanthanum manganite (LSM) electrodes have been the material of choice for cathodes in high temperature solid oxide fuel cells (SOFCs). LSM has relatively high electrical conductivity at high temperatures and has mechanical properties that are well matched to yttria stabilized zirconia (YSZ), a common electrolyte material. Recently, LSM electrodes have been employed in lower temperature (300-500 °C) electrochemical gas purification applications. Several studies have attributed the electrochemical activation of LSM electrodes to changes in the surface stoichiometry under an applied potential.1-3 The presented work explores the polarisation induced changes in LSM electrode composition by utilizing in operando Raman spectroscopy and post mortem ToF-SIMS depth profiling on LSM thin film model electrodes fabricated by pulsed laser deposition on YSZ substrates with a thin (200 nm) CGO barrier layer. Experiments were conducted on cells with 200 nm thick (La0.85Sr0.15)0.9MnO3±δ electrodes in 10% O2 at 500°C and 700°C under various electrical polarisations (-0.5V, ±1V and -2.5V). Raman spectra recorded continuously during polarisation showed evidence of shifts in band intensities that were both reversible and dependent on the direction of the applied potential (Figure 1). The spectral changes were assigned to changes in the LSM electronic structure and specifically to changes in the relative oxide concentration in LSM’s near surface region. Ex situ ToF-SIMS depth profiles were recorded through the LSM thin film electrodes and revealed distinct compositional changes throughout the electrodes (Figure 2). The electrode elements and impurities separated into distinct layers that were more pronounced for the stronger applied polarisations. The mechanism behind this separation into “layers” in the LSM electrode poses interesting questions about mass transfer and ion migration in conducting materials subject to electrical polarisation.

Figure 1. Representative Raman spectra collected on an LSM electrode at 700 °C with the cell open at circuit voltage (OCV) and polarised at (a) -1 V and (b) +1 V. The peaks at 440 and 600 cm⁻¹ are signatures from the CGO and YSZ electrolyte, respectively. Figure 2. ToF-SIMS depth profile of LSM electrode polarised at -1V at 700 °C for 2 h. Stapled lines mark layers enriched in different species. References 1 M. Backhaus-Ricoult, K. Adib, T. St.Clair, B. Luerssen, L. Gregoratti and A. Barinov, Solid State Ionics, 2008, 179, 891. 2 M. A. Haider and S. McIntosh, J. Electrochem. Soc., 2009, 156, B1369. 3 S. P. Jiang and J. G. Love, Solid State Ionics, 2003, 158, 45. [Figure]
**Preparation and Characterisation of Mg$_{1-x}$Rh$_x$B$_2$**

Mg$_{1-x}$Rh$_x$B$_2$ samples were prepared by mixing the elemental powders and sintering at 800 °C under Ar atmosphere. Magnetisation measurements show that the critical temperature decreases as the nominal content of Rh is increased at an average rate of ~0.8 K/at. %. Energy-dispersive X-ray spectroscopy (EDS) analysis shows that some Rh-enriched phases were formed at high doping levels. Based on these measurements as well as X-ray diffraction patterns, it was determined that Mg can be replaced by Rh up to 2.2–2.5 at. % approximately. Two sets of unidentified reflections appear in the X-ray diffraction patterns from $x = 0.01$ and above $x = 0.020$ respectively. The a-axis and c-axis parameters remain almost constant in the doped samples.
Preparation and characterization of polyacrylamide-modified kaolinite containing poly [acrylic acid-co-methylene bisacrylamide] nanocomposite hydrogels

Novel nanocomposite hydrogel structures based on cross-linked poly(acrylic acid) (PAA) and kaolinite (Kaol), modified with different loadings of polyacrylamide (PAAm), were prepared by inverse dispersion polymerization. Ceric ammonium nitrate as an initiator in the presence of nitric acid was used to graft PAAm from the Kaol surface. The surface-modified Kaol showed enhanced interactions between the filler and the PAA matrix, through interactions between amino (-NH2) from PAAm and carboxylic groups (-COOH) from PAA. The XRD and TEM measurements confirmed the exfoliated nanocomposites with the Kaol filler. The swelling degree (SD) of the swollen hydrogel nanocomposite was increased following the addition of polyacrylamide-modified Kaol particles into the hydrogel structures. Rheological characterization showed that an increase in the storage modulus (G') could be a consequence of a good dispersion of Kaol particles in the polyacrylic acid matrix, thereby leading to enhanced interactions and furthermore to improved mechanical properties of the final hydrogels.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Energy Conversion and Storage, Proton conductors, The Danish Polymer Centre, National Research and Development Institute for Chemistry and Petrochemistry, University of South Toulon-Var, Polytechnic University, Romanian Academy
Authors: Zaharia, A. (Ekstern), Sarbu, A. (Ekstern), Radu, A. (Ekstern), Jankova Atanasova, K. (Intern), Daugaard, A. E. (Intern), Hvilsted, S. (Intern), Perrin, F. (Ekstern), Teodorescu, M. (Ekstern), Munteanu, C. (Ekstern), Fruth-Oprisan, V.
Probing individual subcells of fully printed and coated polymer tandem solar cells using multichromatic opto-electronic characterization methods

In this study, a method to opto-electronically probe the individual junctions and carrier transport across interfaces in fully printed and coated tandem polymer solar cells is described, enabling the identification of efficiency limiting printing/coating defects. The methods used are light beam induced current (LBIC) mapping, External quantum efficiency (EQE) measurements, and monochromatic current-voltage (I-V) characterization. Using these methods, inherent limitations to the accuracy of EQE and LBIC measurements on non-ideal tandem solar cells are identified and described through the use of a small-signal electrical model. The model is able to predict the EQE spectrum of the non-ideal polymer tandem solar cell, using extracted values of shunt- and series resistance of the individual junction of the tandem cell. This finally enables LBIC mapping of the individual junctions of the tandem polymer solar cells, using a combination of light and voltage-biasing.
Promotional effect of phosphorus doping on the activity of the Fe-N/C catalyst for the oxygen reduction reaction

Cost-effective, active and stable electrocatalysts for the oxygen reduction reaction (ORR) are highly desirable for the widespread adoption of technologies such as fuel cells and metal-air batteries. Among the already reported non-precious metal catalysts, carbon-supported transition metal-nitrogen complexes, i.e., M-N/C catalysts, are the most promising candidate.
Herein, by comparing the ORR activities of standard Fe-N/C catalysts synthesized with or without the doped phosphorus species, the promotional effect of phosphorus doping is discerned. Such phosphorus doping is achieved by using an acidic phosphate ester as a dopant in the synthesis, which introduces no change in catalyst morphologies and structures. The linked structure of phosphate ester cations with the nitrogen precursor, i.e., polyaniline chain, is favored for the evenly P doping of the catalyst, showing to a superior ORR activity to that for the undoped Fe-N/C catalyst. The activity and durability of the catalysts are demonstrated in direct methanol fuel cells.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Changchun Institute of Applied Chemistry
Authors: Hu, Y. (Ekstern), Zhu, J. (Ekstern), Lv, Q. (Ekstern), Liu, C. (Ekstern), Li, Q. (Intern), Xing, W. (Ekstern)
Number of pages: 6
Pages: 335-340
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochimica Acta
Volume: 155
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.651 SNIP 1.592 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.621 SNIP 1.803 CiteScore 4.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.691 SNIP 1.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.536 SNIP 1.625
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.533 SNIP 1.47
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.563 SNIP 1.595
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.534 SNIP 1.736
Proton Conducting Fuel Cells where Electrochemistry Meets Material Science

Fuel cells are electrochemical devices which directly convert the chemical energy of fuels into electrical energy. They are featured of high energy conversion efficiency and minimized pollutant emission. Proton conducting electrolytes are primarily used as separator materials for low and intermediate temperature fuel cells. High power density, lower temperature and dynamic modes of operation make the technology attractive for both automobile and stationary applications in particular in association with renewable energy sources. This talk starts with a brief introduction to the technology followed by a review of the state-of-the-art in terms of performance, lifetime and cost. Technically faced challenges are then outlined on a system level and traced back to fundamental issues of the proton conducting mechanisms and materials. Perspectives and future research are sketched from a materials science point of view including novel proton conducting materials and non-precious metal catalysts. The discussion will be made with highlights of DTU’s recent research and of course addressing a diverse technical audience.

Pt-Si Bifunctional Surfaces for CO and Methanol Electro-Oxidation

Bimetallic surfaces offer activity benefits derived from synergistic effects among active sites with uniquely different functions, which is particularly important for the development of highly effective heterogeneous catalysts for specific technological applications, such as energy conversion and storage. Here we report on Pt-Si bulk samples prepared by arc-melting, for the first time, with high activities toward the electro-oxidation of CO and methanol. Increasing the Si concentration on the surface was correlated with the shifts of onset oxidation potentials to lower values and higher activities for CO and methanol electro-oxidation. It is proposed that the reaction on the Pt-Si catalyst could follow a Langmuir-Hinshelwood type of mechanism, where substantially enhanced catalytic activity is attributed to the fine-tuning of the surface Pt-Si atomic structure.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Li, Q. (Intern)
Publication date: 2015
Event: Abstract from Tiltrædelsesforelæsning, Lyngby, Denmark.
Main Research Area: Technical/natural sciences

Bibliographical note
Inaugural Lecture (Professor)
Publication: Communication › Conference abstract for conference – Annual report year: 2016
Pulsed laser deposition from ZnS and Cu$_2$SnS$_3$ multicomponent targets

Thin films of ZnS and Cu$_2$SnS$_3$ have been produced by pulsed laser deposition (PLD), the latter for the first time. The effect of fluence and deposition temperature on the structure and the transmission spectrum as well as the deposition rate has been investigated, as has the stoichiometry of the films transferred from target to substrate. Elemental analysis by energy dispersive X-ray spectroscopy indicates lower S and Sn content in Cu$_2$SnS$_3$ films produced at higher fluence, whereas this trend is not seen in ZnS. The deposition rate of the compound materials measured in atoms per pulse is considerably larger than that of the individual metals, Zn, Cu, and Sn.

General information

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Ettlinger, R. B. (Intern), Cazzaniga, A. C. (Intern), Canulescu, S. (Intern), Pryds, N. (Intern), Schou, J. (Intern)
Pages: 385-390
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Applied Surface Science
Volume: 336
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.951 SNIP 1.225
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.914 SNIP 1.3 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.958 SNIP 1.477 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.965 SNIP 1.488 CiteScore 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.918 SNIP 1.373 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.908 SNIP 1.402 CiteScore 2.27
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.924 SNIP 1.141
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.842 SNIP 1.023
Web of Science (2009): Indexed yes
Quantitative 3D X-ray imaging of densification, delamination and fracture in a micro-composite under compression

Phase-contrast three-dimensional tomograms showing in unprecedented detail the mechanical response of a micro-composite subjected to a mechanical compression test are reported. The X-ray ptychography images reveal the deformation and fracture processes of a 10 μm diameter composite, consisting of a spherical polymer bead coated with a nominally 210 nm metal shell. The beginning delamination of the shell from the core can be directly observed at an engineering strain of a few percent. Pre-existing defects are shown to dictate the deformation behavior of both core and shell. The strain state of the increasingly compressed polymer core is assessed quantitatively through the local densification at sub-micron resolution, supported by finite element analysis. Nanoscale mechanics is of rapidly growing importance in materials science, biotechnology and medicine, and this study demonstrates the use of coherent X-ray microscopy as a powerful tool for in situ studies of the mechanical properties of nanostructured devices, structures, and composites. Ptychographic X-ray microscopy can be used for quantitatively studying the mechanical properties of microscale composites. Phase-contrast three-dimensional tomograms reveal with unprecedented detail the mechanical response, including delamination, densification and fracture, of a polymer-core/silver-shell micro-composite subjected in situ to a mechanical compression test.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Norwegian University of Science and Technology, Paul Scherrer Institut
Authors: Bø Fløystad, J. (Ekstern), Skjønsfjell, E. T. B. (Ekstern), Guizar-Sicairos, M. (Ekstern), Høydalsvik, K. (Ekstern), He, J. (Ekstern), Andreasen, J. W. (Intern), Zhang, Z. (Ekstern), Breiby, D. W. (Ekstern)
Number of pages: 9
Pages: 545-553
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Engineering Materials
Volume: 17
Issue number: 4
ISSN (Print): 1438-1656
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.826 SNIP 1.083
Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.807 SNIP 1.045 CiteScore 1.82
Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.805 SNIP 1.089 CiteScore 1.66
Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.733 SNIP 0.843 CiteScore 1.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes

BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.779 SNIP 0.959 CiteScore 1.46
ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.828 SNIP 1.035 CiteScore 1.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes

BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.097 SNIP 1.14

BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.283 SNIP 1.106

BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.267 SNIP 1.153

Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.014 SNIP 1.157
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.051 SNIP 1.386
Scopus rating (2005): SJR 0.875 SNIP 1.131
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.724 SNIP 0.989
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.943 SNIP 1.35
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.924 SNIP 1.137
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.746 SNIP 1.171
Scopus rating (2000): SJR 0.201 SNIP 0.149

Original language: English

Compression testing, Deformation, Degrees of freedom (mechanics), Delamination, Finite element method, Mechanical properties, Deformation and fracture, Deformation behavior, Engineering strains, Mechanical compression tests, Mechanical response, Spherical polymers, Sub-micron resolutions, Three-dimensional tomograms, Fracture

Electronic versions:
Quantitative_3D_X_ray_Imaging_of_Densification_postprint.pdf

DOIs:
10.1002/adem.201400443

Source: FindIt
Source-ID: 274547127
Publication: Research - peer-review › Journal article – Annual report year: 2015
Reactions and SEI Formation during Charging of Li-O2 Cells

In this letter we combine detailed electrochemical impedance measurements with quantitative measurements of O2 evolution and Li2O2 oxidation to describe the charge mechanisms during charge of Li-O2 batteries with porous carbon electrodes. We identify Li2O2 oxidation at 3.05 V and an apparent chemical formation of a solid electrolyte interface (SEI) layer as the first monolayer of Li2O2 is oxidized, leading to a voltage increase. The first electrochemical degradation reaction is identified between 3.3 V and 3.5 V, and the chemical degradation is limited above 3.5 V, suggesting that a chemically stable SEI layer has been formed.

General information

State: Published
Authors: Højberg, J. (Intern), Knudsen, K. B. (Intern), Hjelm, J. (Intern), Vegge, T. (Intern)
Pages: A63-A66
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: ECS Electrochemistry Letters
Volume: 4
Issue number: 7
ISSN (Print): 1099-0062
Ratings:
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.61 SNIP 0.751 CiteScore 1.76
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.735 SNIP 0.652 CiteScore 1.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.631 SNIP 0.768 CiteScore 1.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.631 SNIP 0.647 CiteScore 1.48
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.064 SNIP 1.006
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.032 SNIP 0.967
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.169 SNIP 1.011
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.227 SNIP 1.001
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.332 SNIP 1.11
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.438 SNIP 1.133
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.474 SNIP 1.225
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.476 SNIP 1.231
Redox Probing Study of the Potential Dependence of Charge Transport Through Li₂O₂

In the field of energy storage devices the pursuit for cheap, high energy density, reliable secondary batteries is at the top of the agenda. The Li–O₂ battery is one of the possible technologies that, in theory, should be able to close the gap, which exists between the present state-of-the-art Lion technologies and the demand placed on batteries by technologies such as electrical vehicles. Here we present a redox probing study of the charge transfer across the main deposition product lithium peroxide, Li₂O₂, in the Li–O₂ battery using outer-sphere redox shuttles. The change in heterogeneous electron transfer exchange rate as a function of the potential and the Li₂O₂ layer thickness (∼depth-of-discharge) was determined using electrochemical impedance spectroscopy. The attenuation of the electron transfer exchange rate with film thickness is dependent on the probing potential, providing evidence that hole transport is the dominant process for charge transfer through Li₂O₂ and showing that the origin of the sudden death observed upon discharge is due to charge transport limitations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Stanford University
Authors: Knudsen, K. B. (Intern), Luntz, A. C. (Ekstern), Jensen, S. H. (Intern), Vegge, T. (Intern), Hjelm, J. (Intern)
Number of pages: 8
Pages: 28292–28299
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Volume: 119
Issue number: 51
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Reduced graphene oxide for Li–air batteries: the effect of oxidation time and reduction conditions for graphene oxide

Reduced graphene oxide (rGO) has shown great promise as an air-cathode for Li-air batteries with high capacity. In this article we demonstrate how the oxidation time of graphene oxide (GO) affects the ratio of different functional groups and how trends of these in GO are extended to chemically and thermally reduced GO. We investigate how differences in functional groups and synthesis may affect the performance of Li-O-2 batteries. The oxidation timescale of the GO was varied between 30 min and 3 days before reduction. Powder X-ray diffraction, micro-Raman, FE-SEM, BET analysis, and XPS were used to characterize the GO's and rGO's. Selected samples of GO and rGO were analyzed by solid state C-13 MAS NMR. These methods highlighted the difference between the two types of rGO's, and XPS indicated how the chemical trends in GO are extended to rGO. A comparison between XPS and C-13 MAS NMR showed that both techniques can enhance the structural understanding of rGO. Different rGO cathodes were tested in Li-O-2 batteries which revealed a difference in overpotentials and discharge capacities for the different rGO's. We report the highest Li-O-2 battery discharge capacity recorded of approximately 60,000 mAh/gcarbon achieved with a thermally reduced GO cathode. (C) 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Copenhagen, University of Southern Denmark, Uppsala University
Number of pages: 12
Pages: 233-244
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Reducing Systematic Errors in Oxide Species with Density Functional Theory Calculations

Density functional theory calculations can be used to gain valuable insight into the fundamental reaction processes in metal–oxygen systems, e.g., metal–oxygen batteries. Here, the ability of a range of different exchange-correlation functionals to reproduce experimental enthalpies of formation for different types of alkali and alkaline earth metal oxide species has been examined. Most examined functionals result in significant overestimation of the stability of superoxide species compared to peroxides and monoxides, which can result in erroneous prediction of reaction pathways. We show that if metal chlorides are used as reference structures instead of metals, the systematic errors are significantly reduced and functional variations decreased. Using a metal chloride reference, where the metal atoms are in the same oxidation state as in the oxide species, will provide a computationally inexpensive and robust approach to significantly improve accuracy. The approach can potentially be applied to improve accuracy of calculations more generally.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, SLAC National Accelerator Laboratory
Authors: Christensen, R. (Intern), Hummelshøj, J. S. (Ekstern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 17596–17601
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Volume: 119
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Reduction of a Ni/Spinel Catalyst for Methane Reforming

A nickel/spinel (Ni/MgAl2O4) catalyst, w(Ni) = 22 wt%, was investigated in situ during reduction with wide angle X-ray scattering (WAXS) in a laboratory setup and with anomalous small angle X-ray scattering (ASAXS) at a synchrotron source. Complementary high resolution transmission electron microscopy (HRTEM) was performed on the fresh catalyst sample. The Ni particles in the fresh catalyst sample were observed to exhibit a Ni/NiO core/shell structure. A decrease of the Ni lattice parameter is observed during the reduction in a temperature interval from 413 – 453 K, which can be related to the reduction of the NiO shell, whereby stress due to the lattice mismatch of Ni and NiO is relieved.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Individual Nanoparticle Functionality, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Experimental Surface and Nanomaterials Physics, Atomic scale modelling and materials, Norwegian University of Science and Technology, California Institute of Technology, Haldor Topsoe AS
Pages: 1424–1432
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Volume: 119
Issue number: 3
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
RES Hydrogen: efficient pressurised alkaline electrolysers
The RESelyser project addresses issues associated with coupling alkaline electrolysis to renewable energy sources such as electrode stability and gas purity by implementing improved electrodes and a new separator membrane concept. The project aims to improve performance, operation pressure and reduce system cost. The project supports DTU Energy’s activities on electrodes within the larger FCH-JU project. The overall project demonstrated: improved electrode efficiency also during cyclic operation, safe gas purity at a system pressure of 30 bar, 10 kW stack operation and estimated system costs including BoP. Investigation of cathodes revealed highly heterogeneous microstructures and 3D microstructure quantification methods were developed. Nanometre scale -Ni(OH)2 formation was identified on tested cathode surfaces and is considered a potential degradation mechanism that is not presently well understood.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bowen, J. R. (Intern), Bentzen, J. J. (Intern), Jørgensen, P. S. (Intern), Zhang, W. (Intern)
Number of pages: 48
Publication date: 2015

Publication information
Publisher: DTU Energy Conversion
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
RES_Hydrogen.pdf
Links:
http://energiforskning.dk/node/7012

Bibliographical note
Final report to Energinet.dk for RESelyser project. Report is available from http://energiforskning.dk/node/7012. Please make link to the RESelyser project in ORBIT. Co-authors are listed on page 2 of report.
Residual stresses and strength of multilayer tape cast solid oxide fuel and electrolysis half-cells

The cost-effectiveness of Solid Oxide Cells production can be improved by introducing "multilayer-tape-casting" (MTC: sequential casting of the layers) and co-sintering of the half-cells. MTC additionally results in more homogeneous layers with strong interfaces. However, the thermal expansion coefficient (TEC) mismatch between the layers, cumulated from high temperature, induces significant residual stresses in the half-cells. Furthermore, it has been observed that MTC half-cells with 4 layers (MTC4: support, fuel electrode, electrolyte and barrier layer) are sometimes more fragile to handle than those with 3 layers (MTC3: without barrier layer). The bending strength of MTC3 and MTC4 under various loading orientations (electrolyte on the tensile or compressive side of the loading) is compared. The analysis, by taking residual stresses into account, shows that the strength of the half-cells with the electrolyte on the compressive side corresponds to the strength of the support. With the loading in the other direction (electrolyte on the tensile side), the origin of the failure is in a different layer for MTC3 (fuel electrode) and for MTC4 (barrier layer). In order to decrease the tensile residual stresses, especially in the outer barrier-layer, possible changes to the layer properties are discussed and some optimization guidelines proposed.
Rheological properties of poly(vinylpyrrolidone) as a function of average molecular weight and its applications

Polyvinylpyrrolidone (PVP) is an attractive material due to its solubility in aqueous and organic solvents, excellent film forming capability, and its ability to act as a dispersant in colloidal suspensions and slurries. These characteristics of PVP have led to its use in a large variety of formulations for pharmaceutics, food, personal care, or coatings, paintings, and printing applications. It is also widely used as an organic additive, i.e., dispersant for ceramics. Regardless of the application, the control over the polymer behavior in solution is required for an efficient optimization of the formulation. Specifically, understanding the rheological properties is of paramount interest. Among the different factors that influence the rheological behavior, viscosity average molecular weight of the polymer is the most relevant. In this work, PVP polymers with various molecular weights have been characterized regarding their viscosimetric properties in ethanol. Average molecular weights (Mw, Mn, and Mz) have been determined by gel permeation chromatography (GPC), and then used in a numerical method to evaluate the viscosity average molecular weight (Mv) via the Mark-Houwink-Sakurada (MHS) equation. The MHS equation relates the intrinsic viscosity [η] of a polymer in a given solvent at fixed temperature to the molecular weight. The adopted method also enables for the evaluation of the two MHS equation parameters (a and K), and of the polydispersity correction factor (qMHS). The intrinsic viscosity, which is the inherent ability of a solute to increase the viscosity of a solvent, used in the MHS equation, has been evaluated via the dilution method. The knowledge obtained from this fundamental study on PVP behavior, has been successfully applied to different case studies.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Self-Organized Nanoporous Materials
Authors: Marani, D. (Intern), Sudireddy, B. R. (Intern), Kiebach, R. (Intern), Nielsen, L. (Intern), Ndoni, S. (Intern)
Publication date: 2015
Event: Abstract from 1st Annual World Congress of Smart Materials 2015, Busan, Korea, Republic of.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015
Role of Li$_2$O$_2$@Li$_2$CO$_3$ Interfaces on Charge Transport in Nonaqueous Li–Air Batteries

The formation and oxidation of the main discharge product in nonaqueous secondary Li–O$_2$ batteries, that is, Li$_2$O$_2$, has been studied intensively, but less attention has been given to the formation of cathode–electrolyte interfaces, which can significantly influence the performance of the Li–O$_2$ battery. Here we apply density functional theory with the Hubbard U correction (DFT+U) and nonequilibrium Green’s function (NEGF) methods to investigate the role of Li$_2$O$_2$@Li$_2$CO$_3$ interface layers on the ionic and electronic transport properties at the oxygen electrode. We show that, for example, lithium vacancies accumulate at the peroxide part of the interface during charge, reducing the coherent electron transport by two to three orders of magnitude compared with pristine Li$_2$O$_2$. During discharge, Li$_2$O$_2$@Li$_2$CO$_3$ interfaces may, however, provide an alternative in-plane channel for fast electron polaron hopping that could improve the electronic conductivity and ultimately increase the practical capacity in nonaqueous Li–O$_2$ batteries.
Roll and roll-to-roll process scaling through development of a compact flexo unit for printing of back electrodes

We report manufacture of fully printed and coated polymer solar cells on a small scale roll-to-roll coater representing the intermediate scale between laboratory and pilot scale. We highlight the enormous span in scale between the laboratory scale and the intended industrial scale by a factor of >100,000 and detail how this enormous scale must be covered by equipment that follow the scale. Especially the intermediate scale between equipment that can fit inside a fume cupboard and the typical pilot equipment with a footprint having the size of a large room presents a challenge that comprises some of the most critical steps in the scaling process. We describe the development of such a machine that comprise web guiding, tension control and surface treatment in a compact desk size that is easily moved around and also detail the development of a small cassette based flexographic unit for back electrode printing that is parsimonious in terms of ink usage and more gentle than laboratory scale flexo units where the foil transport is either driven by the flexo unit or the flexo unit is driven by the foil transport. We demonstrate fully operational flexible polymer solar cell manufacture using this new roll and roll-to-roll (R3) approach and compare with the existing methods.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Grafisk Maskinfabrik A/S
Authors: Dam, H. F. (Intern), Andersen, T. R. (Intern), Madsen, M. V. (Intern), Mortensen, T. K. (Ekstern), Pedersen, M. F. (Ekstern), Nielsen, U. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 6
Pages: 187-192
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 140
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
Roll-Coated Fabrication of Fullerene-Free Organic Solar Cells with Improved Stability

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Chinese Academy of Sciences, Zhejiang University
Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences
Roll-coating fabrication of ITO-free flexible solar cells based on a non-fullerene small molecule acceptor

We report organic solar cells (OSCs) with non-fullerene small molecule acceptors (SMAs) prepared in large area via a roll coating process. We employ all solution-processed indium tin oxide (ITO)-free flexible substrates for inverted solar cells with a new SMA of F(DPP)(2)B-2. By utilizing poly(3-hexylthiophene) as donor blended with F(DPP)(2)B-2 as acceptor, ITO-free large-area flexible SMA based OSCs were produced under ambient conditions with the use of slot-die coating and flexographic printing methods on a lab-scale compact roll-coater that is readily transferrable to roll-to-roll processing. The effect of different processing solvents on the device performance was investigated, and the best performance with a power conversion efficiency of 0.65%, an open circuit voltage of 0.85 V, a short-circuit current density of 2.19 mA cm(-2), and a fill factor of 35% was obtained.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Zhejiang University, Chinese Academy of Sciences, Peking University
Number of pages: 6
Pages: 36001-36006
Publication date: 2015
Main Research Area: Technical/natural sciences
Roll-to-Roll Printed Silver Nanowire Semitransparent Electrodes for Fully Ambient Solution-Processed Tandem Polymer Solar Cells

Silver nanowires (AgNWs) and zinc oxide (ZnO) are deposited on flexible substrates using fast roll-to-roll (R2R) processing. The AgNW film on polyethylene terephthalate (PET) shows >80% uniform optical transmission in the range of 550-900 nm. This electrode is compared to the previously reported and currently widely produced indium-tin-oxide (ITO) replacement comprising polyethylene terephthalate (PET)|silver grid|poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS)|ZnO known as Flextrode. The AgNW/ZnO electrode shows higher transmission than Flextrode above 490 nm in the electromagnetic spectrum reaching up to 40% increased transmission at 750 nm in comparison to Flextrode. The functionality of AgNW electrodes is demonstrated in single and tandem polymer solar cells and compared with parallel devices on traditional Flextrode. All layers, apart from the semitransparent electrodes which are large-scale R2R produced, are fabricated in ambient conditions on a laboratory roll-coater using printing and coating methods which are directly transferrable to large-scale R2R processing upon availability of materials. In a single cell structure, Flextrode is preferable with active layers based on poly-3-hexylthiophene(P3HT);phenyl-C61-butyric acid methylester (PCBM) and donor polymers of similar absorption characteristics while AgNW/ZnO electrodes are more compatible with low band gap polymer-based single cells. In tandem devices, AgNW/ZnO is more preferable resulting in up to 80% improvement in PCE compared to parallel devices on Flextrode. Rolling in tandem: Roll-to-roll rotary screen printing of silver nanowires (AgNWs) and zinc oxide (ZnO) is realized on flexible substrates enabling large-area semi-transparent electrodes with >80% transmission. This electrode is employed in all-ambient roll-coating of single and tandem polymer solar cells. AgNW/ZnO proves highly suitable especially for tandem structures while the traditional indium-tin-oxide replacement - Flextrode - remains unbeaten in single cells with wide band-gap polymers.
Round-Robin Studies on Roll-Processed ITO-free Organic Tandem Solar Cells Combined with Inter-Laboratory Stability Studies

Roll-processed, indium tin oxide (ITO)-free, flexible, organic tandem solar cells and modules have been realized and used in round-robin studies as well as in parallel inter-laboratory stability studies. The tandem cells/modules show no significant difference in comparison to their single-junction counterparts and the use of round-robin studies as a consensus tool for evaluation of organic solar cell parameters is judged just as viable for the tandem solar cells as for single-junction devices. The inter-laboratory stability studies were conducted according to testing protocols ISOS-D-2, ISOS-D-3, and ISOS-L-2, and in spite of a much more complicated architecture the organic tandem solar cells show no significant difference in stability in comparison to their single-junction counterparts.

General information
State: Published
Pages: 423-427
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Technology
Volume: 3
Issue number: 4
ISSN (Print): 2194-4288
Ratings:
Web of Science (2017): Indexed yes
Scopus rating (2016): SJR 0.283 SNIP 0.13 CiteScore 0.66
Scopus rating (2015): SNIP 0.103 SJR 0.163 CiteScore 0.21
Web of Science (2015): Indexed yes
Scopus rating (2014): SNIP 0.564 SJR 1.681
Web of Science (2014): Indexed yes
ISI indexed (2013): ISI indexed no
Original language: English
Scalable single point power extraction for compact mobile and stand-alone solar harvesting power sources based on fully printed organic photovoltaic modules and efficient high voltage DC/DC conversion

Patterns for fully printed polymer solar cells are presented that inherently enable scaling of the power output with single point electrical energy connection is presented. Connection is made to only one end of the printed foil that can be rolled out for light energy harvesting. The power level is simply increased/decreased by increasing/decreasing the length of the foil with a corresponding increase/decrease in operating voltage. The current flow runs in both directions along the printed foil thus alleviating the need for post process addition of complex busbar topologies. The power conversion takes place in a HVDC–DC converter that is tailored specifically for operation with polymer solar cells by regulation on the input side. The system charges a lithium-polymer battery thus enabling storage of 82 Wh for a printed OPV foil measuring 0.305 m×9 m having a nominal power output of at least 15 W (AM1.5G, 1000 W m⁻²). As a demonstration we present a scalable fully integrated and compact power unit for mobile applications comprising solar energy harvesting OPV modules, power conversion and storage. Applications possible include electrical charging of mobile devices, illumination using LED lamps and low mechanical power applications such as pumping water.
Segmentation of low-cost high efficiency oxide-based thermoelectric materials

Thermoelectric (TE) oxide materials have attracted great interest in advanced renewable energy research owing to the fact that they consist of abundant elements, can be manufactured by low-cost processing, sustain high temperatures, be robust and provide long lifetime. However, the low conversion efficiency of TE oxides has been a major drawback limiting these materials to broaden applications. In this work, theoretical calculations are used to predict how segmentation of oxide and semimetal materials, utilizing the benefits of both types of materials, can provide high efficiency, high temperature oxide-based segmented legs. The materials for segmentation are selected by their compatibility factors and their conversion efficiency versus material cost, i.e., "efficiency ratio". Numerical modelling results showed that conversion efficiency could reach values of more than 10% for unicouples using segmented legs based p-type Ca$_3$Co$_4$O$_9$ and n-type ZnO oxides excluding electrical and thermal losses. It is found that the maximum efficiency of segmented unicouple could be linearly decreased with increasing the interfacial contact resistance. The obtained results provide useful tool for designing a low-cost and high efficiency thermoelectric modules based-oxide materials.
Segmented Thermoelectric Oxide-Based Module for High-Temperature Waste Heat Harvesting

We report a high-performance thermoelectric (TE) oxide-based module using the segmentation of half-Heusler Ti_{0.3}Zr_{0.35}Hf_{0.35}CoSb_{0.8}Sn_{0.2} and misfit-layered cobaltite Ca_{3}Co_{4}O_{9+δ} as the p-leg and 2% Al-doped ZnO as the n-leg. The maximum output power of a 4-couple segmented module at ΔT=700 K attains a value of approximately 6.5 kWm⁻², which is three times higher than that of the best reported non-segmented oxide module. The TE properties of individual legs, as well as the interfacial contact resistances, were characterized as a function of temperature. Numerical modeling was used to predict the efficiency and to evaluate the influence of the electrical and thermal losses on the performance of TE modules. Initial long-term stability tests of the module at the hot and the cold side temperatures of 1073 K and 444 K, respectively, showed a promising result with 4% degradation for 48 h operating in air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Johannes Gutenberg University, California Institute of Technology
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Number of pages: 10
Pages: 1143–1151
Publication date: 2015
Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation

Water is a life-giving source, fundamental to human existence, yet over a billion people lack access to clean drinking water. The present techniques for water treatment such as piped, treated water rely on time and resource intensive centralized solutions. In this work, we propose a decentralized device concept that can utilize sunlight to split water into hydrogen and hydrogen peroxide. The hydrogen peroxide can oxidize organics while the hydrogen bubbles out. In enabling this device, we require an electrocatalyst that can oxidize water while suppressing the thermodynamically favored oxygen evolution and form hydrogen peroxide. Using density functional theory calculations, we show that the free energy of adsorbed OH* can be used to determine selectivity trends between the 2e(-) water oxidation to H2O2 and the 4e(-) oxidation to O2. We show that materials which bind oxygen intermediates sufficiently weakly, such as SnO2, can activate hydrogen peroxide evolution. We present a rational design principle for the selectivity in electrochemical water oxidation and identify new material candidates that could perform H2O2 evolution selectively.
We present simulation results of multi-layer active magnetic regenerators using the solid-state refrigerant La(Fe,Mn,Si)_{13}H_y. This material presents a large, however quite sharp, isothermal entropy change that requires a careful choice of number of layers and working temperature for multi-layer regenerators. The impact of the number of layers and the sensitivity to the working temperature as well as the temperature span are quantified using a one dimensional numerical model. A study of the sensitivity of variation in Curie temperature through a uniform and normal distribution is also presented. The results show that the nominal cooling power is very sensitive to the Curie temperature variation in the multi-layer regenerators. A standard deviation of the Curie temperature variation for a normal distribution less than 0.6 K is suggested in order to achieve sufficient performance of a 15-layer regenerator with Curie temperature spacing of 2 K.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Physics
Volume: 118
Issue number: 1
Article number: 014903
ISSN (Print): 0021-8979
Ratings:
Shape recovery of viscoelastic beams after stowage

The deployment of viscoelastic structures that have been held stowed for a given time duration can be formulated as a viscoelastic boundary value problem in which the prescribed condition switches from constant displacement to constant traction. This paper presents closed-form expressions for the load relaxation and shape recovery of a linear viscoelastic beam subject to such time-varying constraints. It is shown that a viscoelastic beam recovers to its original shape asymptotically over time. The analytical solutions are employed to investigate the effect of temperature and stowage time on the time required to achieve recovery with a specified precision. Based on the time-temperature equivalence principle, the relationship between recovery time and holding duration is concisely presented on a single plot. It is found that recovery time increases with holding duration but with a diminishing effect.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Kwok, K. (Intern)
Pages: 95-111
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Mechanics Based Design of Structures and Machines
Volume: 43
Issue number: 1
ISSN (Print): 1539-7734
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.556 SNIP 0.991 CiteScore 1.63
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.631 SNIP 1.48 CiteScore 1.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.754 SNIP 1.559 CiteScore 1.17
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.52 SNIP 0.984 CiteScore 0.92
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.403 SNIP 0.658 CiteScore 0.61
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.213 SNIP 0.697 CiteScore 0.49
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.345 SNIP 0.864
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.593 SNIP 0.626
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.304 SNIP 0.559
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.199 SNIP 0.381
Scopus rating (2006): SJR 0.384 SNIP 0.626
Scopus rating (2005): SJR 0.243 SNIP 0.583
Scopus rating (2004): SJR 0.323 SNIP 0.613
Significant Electronic Thermal Transport in the Conducting Polymer Poly(3,4-ethylenedioxythiophene)

Suspended microdevices are employed to measure the in-plane electrical conductivity, thermal conductivity, and Seebeck coefficient of suspended poly(3,4-ethylenedioxythiophene) (PEDOT) thin films. The measured thermal conductivity is higher than previously reported for PEDOT and generally increases with the electrical conductivity. The increase exceeds that predicted by the Wiedemann–Franz law for metals and can be explained by significant electronic thermal transport in PEDOT.
Size of oxide vacancies in fluorite and perovskite structured oxides

An analysis of the effective radii of vacancies and the stoichiometric expansion coefficient is performed on metal oxides with fluorite and perovskite structures. Using the hard sphere model with Shannon ion radii we find that the effective radius of the oxide vacancy in fluorites increases with increasing ion radius of the host cation and that it is significantly smaller than the radius of the oxide ion in all cases, from 37% smaller for HfO₂ to 13% smaller for ThO₂. The perovskite structured LaGaO₃ doped with Sr or Mg or both is analyzed in some detail. The results show that the effective radius of an oxide vacancy in doped LaGaO₃ is only about 6% smaller than the oxide ion. In spite of this the stoichiometric expansion coefficient (a kind of chemical expansion coefficient) of the similar perovskite, LaCrO₃, is significantly smaller than the stoichiometric expansion coefficient of the fluorite structured CeO₂. Our analysis results indicate that the smaller stoichiometric expansion coefficient of the perovskites is associated with the restraining action of the A-O sub-lattice to dimensional changes in the B-O sub-lattice and vice versa.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Atomic scale modelling and materials, Mixed Conductors
Authors: Chatzichristodoulou, C. (Intern), Norby, P. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Number of pages: 8
Pages: 100-107
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Electroceramics
Volume: 34
Issue number: 1
ISSN (Print): 1385-3449
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.15 SJR 0.429 SNIP 0.561
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.568 SNIP 0.761 CiteScore 1.49
Web of Science (2015): Indexed yes
Solid Oxide Cell and Stack Testing, Safety and Quality Assurance (SOCTESQA)

The market penetration of fuel and electrolysis cell energy systems in Europe requires the development of reliable assessment, testing and prediction of performance and durability of solid oxide cells and stacks (SOC). To advance in this field the EU-project “SOCTESQA” was launched in May 2014. Partners from different countries in Europe and one external party from Singapore are working together to develop uniform and industry wide test procedures and protocols for SOC cell/stack assembly. In this project new application fields which are based on the operation of the SOC cell/stack assembly in the fuel cell (SOFC), in the electrolysis (SOEC) and in the reversible SOFC/SOEC mode are addressed. This covers the wide field of power generation systems, e.g. stationary SOFC μ-CHP, mobile SOFC APU and SOFC/SOEC power-to-gas systems. The paper presents the results which have been achieved so far in the SOCTESQA project. Besides a summary of existing test procedures a so called “test matrix” was created. This document includes generic test modules, e.g. current-voltage curves, electrochemical impedance spectroscopy, thermal cycling, electrical current cycling and long term tests both under steady state and dynamic operating conditions. The application specific test programs are created by combining several of these test modules. In a next step defined test modules will be applied for the initial test bench validation, which will be improved by several validation loops. The final test protocols will be confirmed by round robin tests.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, German Aerospace Center, University of Grenoble, Italian National Agency for New Technologies, European Commission - Joint Research Center
Authors: Auer, C. (Ekstern), Lang, M. (Ekstern), Couturier, K. (Ekstern), Ravn Nielsen, E. (Intern), J. McPhail, S. (Ekstern), Tsotridis, G. (Ekstern), Fu, Q. (Ekstern), H. Chan, S. (Ekstern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Solid Oxide Cell and Stack Testing, Safety and Quality Assurance (SOCTESQA)

In the EU-funded project “SOCTESQA” partners from Europe and Singapore are working together to develop uniform and industry wide test procedures and protocols for solid oxide cells and stacks SOC cell/stack assembly. New application fields which are based on the operation of the SOC cell/stack assembly in the fuel cell (SOFC), in the electrolysis (SOEC) and in the combined SOFC/SOEC mode are addressed. This covers the wide field of power generation systems, e.g. stationary SOFC μ-CHP, mobile SOFC APU and SOFC/SOEC power-to-gas systems. This paper presents the results which have been achieved so far. Besides a summary of existing test procedures a so called “test matrix” was created. This document includes generic test modules, e.g. current-voltage curves, electrochemical impedance spectroscopy, thermal cycling, electrical current cycling and long-term tests both under steady-state and dynamic operating conditions. The application specific test programs are created by combining several of these test modules.

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General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, German Aerospace Center, University of Grenoble, Italian National Agency for New Technologies, European Commission - Joint Research Center,
Solid solution barium–strontium chlorides with tunable ammonia desorption properties and superior storage capacity

Metal halide ammines are very attractive materials for ammonia absorption and storage—applications where the practically accessible or usable gravimetric and volumetric storage densities are of critical importance. Here we present, that by combining advanced computational materials prediction with spray drying and in situ thermogravimetric and structural characterization, we synthesize a range of new, stable barium-strontium chloride solid solutions with superior ammonia storage densities. By tuning the barium/strontium ratio, different crystallographic phases and compositions can be obtained with different ammonia ab- and desorption properties. In particular it is shown, that in the molar range of 35–50% barium and 65–50% strontium, stable materials can be produced with a practically usable ammonia density (both volumetric and gravimetric) that is higher than any of the pure metal halides, and with a practically accessible volumetric ammonia densities in excess of 99% of liquid ammonia.
Solution and vapour deposited lead perovskite solar cells: Ecotoxicity from a life cycle assessment perspective

We present a life cycle analysis (LCA) and an environmental impact analysis (EIA) of lead based perovskite solar cells prepared according to the two most successfully reported literature methods that comprise either vapour phase deposition or solution phase deposition. We have developed the inventory for all the components employed for the two different device architectures that resemble respectively a traditional dye sensitised solar cell (DSSC) and an inverted polymer solar cell (OPV). We analyse the impacts from generation of 1 kWh of electricity and assume a lifetime of 1 year in the analysis and further present a sensitivity analysis with the operational lifetime as a basis. We find that the major impact comes from the preparation of the perovskite absorber layer due to the electrical energy required in the manufacture and also make the striking observation that the impact of toxic lead(II)halides is very limited compared to methylammoniumhalides employed. This applies during the raw materials extraction, synthesis of the starting materials and manufacture of the perovskite solar cells and from these points of view the lead based perovskite solar cells do not pose extra concerns when compared to contending solar cell technologies in the cradle-to-gate scenario considered here. The environmental impact of the perovskite solar cells in the operational phase and the decommissioning phase representing a cradle-to-grave analysis is not currently possible and will have to await large scale outdoor demonstration where emission to the environment during the operation and decommissioning phase can be measured. The main conclusion is that in the cradle-to-gate analysis there are no compelling reasons to dismiss lead based perovskites as a solar cell technology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technical University of Cartagena
Authors: Espinosa Martinez, N. (Intern), Serrano-Luján, L. (Ekstern), Urbina, A. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 8
Pages: 303-310
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 137
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.524 SNIP 2.121
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.991 SNIP 1.977
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.654 SNIP 1.458
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.359 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.447 SNIP 1.799
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.141 SNIP 1.619
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.932 SNIP 1.178
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.992 SNIP 1.34
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.042 SNIP 1.114
Scopus rating (2001): SJR 0.896 SNIP 1.235
Scopus rating (2000): SJR 0.828 SNIP 0.986
Scopus rating (1999): SJR 0.701 SNIP 0.75
Space-confined preparation of high surface area tungsten oxide and tungsten nitride inside the pores of mesoporous silica SBA-15

For the direct preparation of high surface area nitride materials, a lack of suitable precursors exists. Indirect preparation by gas phase nitridation (e.g. by ammonia) requires high temperatures and often results in sintering. The present work demonstrates that the space-confined preparation of W2N inside the pores of ordered mesoporous silica SBA-15 offers a possibility to reduce sintering phenomena and thus to obtain smaller particles, porous structures and a higher surface area material. The preparation was pursued in a two-step approach. First, WO3 was introduced into the channels of SBA-15 and second, ammonolysis was conducted for its conversion to W2N. When performed in the presence of the exo-template, SBA-15 acts as a stabilizer and small W2N particles (6-7 nm) with a high specific surface area (40 m² g⁻¹) are obtained after template removal. When the template is, however, removed before nitridation, it cannot stabilize the W2N particles and enhanced sintering occurs. (C) 2015 Elsevier Inc. All rights reserved.
Specific Electrical Conductivity in Molten Potassium Dihydrogen Phosphate KH2PO4 Electrolyte at ~300 °C

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry
Authors: Nikiforov, A. V. (Intern), Berg, R. W. (Intern), Bjerrum, N. J. (Intern)
Pages: 204-204
Publication date: 2015
Conference: The 228th ECS Meeting, Phoenix, Arizona, United States, 11/10/2015 - 11/10/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-02
Issue number: 1
Article number: 4
ISSN (Print): 2151-2043
Original language: English
Links:
https://ecs.confex.com/ecs/228/webprogram/Paper58458.html
Source: FindIt
Source-ID: 276169798
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

Stability of La0.6Sr0.4Co0.2Fe0.8O3/Co0.9Gd0.1O2 cathodes during sintering and solid oxide fuel cell operation
Degradation phenomena of La0.58Sr0.4Co0.2Fe0.8O3/Co0.9Gd0.1O2 (LSCF/CGO) cathodes were investigated via post-mortem analyses of an experimental solid oxide fuel cell (SOFC) stack tested at 700 °C for 2000 h using advanced electron microscopy (SEM-EDS, HR-TEM-EDS) and time-of-flight secondary ion mass spectrometry (TOF-SIMS). Similar studies were carried out on non-tested reference cells for comparison. The analysis focused on the LSCF/CGO cathode
and the CGO barrier layer, as the cathode degradation can be a major contributor to the overall degradation in this type of SOFC. SEM-EDS and TOF-SIMS were used to investigate inter-diffusion across the barrier layer - electrolyte interface and the barrier layer - cathode interface. In addition, TOF-SIMS data were employed to investigate impurity distribution before and after testing. HR-TEM-EDS was used to investigate possible phase segregation in the LSCF and to look for reaction between the phases. The results show that phase separation and inter-diffusion across the cathode-barrier layer interface and the barrier layer-electrolyte interface happened mainly during sintering and cathode firing, and to a very little degree during the test period.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Topsoe Fuel Cell
Pages: 151-161
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 283
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.945 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.297 SNIP 1.981
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.968 SNIP 1.726
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.597 SNIP 1.489
Web of Science (2007): Indexed yes
Stabilized thin film heterostructure for electrochemical applications.
The invention provides a method for the formation of a thin film multi-layered heterostructure upon a substrate, said method comprising the steps of: a. providing a substrate; b. depositing a buffer layer upon said substrate, said buffer layer being a layer of stable ionic conductor (B); c. depositing a layer A upon said buffer layer, said layer A being a layer of fast ionic conductor (A), said layer A having a thickness (tA) of 20 nm or less; d. depositing a layer B upon said layer A, said layer B being a layer of stable ionic conductor (B), said layer B having a thickness (tB) of 150 nm or less; and e. repeating steps b. and c. a total of N times, such that N repeating pairs of layers (A/B) are built up, wherein N is 1 or more. The invention also provides a thin film multi-layered heterostructure as such, and the combination of a thin film multi-layered heterostructure and a substrate. The heterostructure finds use as an electroceramic, in particular in SOFCs.
give us to obtain clear diffraction patterns with high intensity during electrochemical reaction in a short period of time without further relaxation step. We carefully scrutinized reversible structural phase transformations during electrochemical reaction of P2 and O3-layered compounds based on in situ analysis, and detailed results will be discussed.

**General information**
State: Published
Organisations: Department of Chemistry, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Korea Advanced Institute of Science & Technology
Authors: Jung, Y. H. (Ekstern), Christiansen, A. S. (Intern), Johnsen, R. (Intern), Norby, P. (Intern), Kim, D. K. (Ekstern)
Number of pages: 1
Pages: 225
Publication date: 2015
Conference: The 228th ECS Meeting , Phoenix, Arizona, United States, 11/10/2015 - 11/10/2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-02
Issue number: 3
ISSN (Print): 2151-2043
Original language: English
Source: Findit
Source-ID: 276168793
Publication: Research - peer-review » Journal article – Annual report year: 2015

Structure and crystallinity of water dispersible photoactive nanoparticles for organic solar cells
Water based inks would be a strong advantage for large scale production of organic photovoltaic devices. Formation of water dispersible nanoparticles produced by the Landfester method is a promising route to achieve such inks. We provide new insights into the key ink properties of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) nanoparticles such as the internal structure and crystallinity of the dispersed nanoparticles and the previously unreported drastic changes that occur when the inks are cast into a film. We observe through transmission electron microscopy (TEM) and small angle X-ray scattering (SAXS) that the nanoparticles in dispersion are spherical with the nanodomains of P3HT being partly crystalline. When wet processed and dried into films, the nanoparticles lose their spherical shape and become flattened into oblate shapes with a large aspect ratio. Most particles are observed to have a diameter 13 times of the particle height. After casting into a film, the crystal domains adopt a preferred orientation with the majority of the nanocrystals (68%) with face-on orientation to the substrate. We propose that low substrate surface energy is responsible for particle deformation and texturing.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Functional organic materials, University of Copenhagen, Aalborg University, Changchun Institute of Applied Chemistry
Pages: 17022-17031
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 33
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Studies on the thermal decomposition of lanthanum(III) valerate and lanthanum(III) caproate in argon

The decomposition of La-valerate (La(C4H9CO2)3·xH2O (x ≈ 0.45)) and La-caproate (La(C5H11CO2)3·xH2O (x ≈ 0.30)) was studied upon heating at 5°C/min in a flow of argon. Using a variety of techniques including simultaneous TG-DTA, FTIR, X-ray diffraction with both laboratory Cu Kα and synchrotron sources as well as hot-stage microscopy, it was found that both compounds melt prior to decomposition and that the main decomposition stage from the molten, anhydrous state leads to the formation of La-dioxycarbonate (La2O2CO3) via an unstable intermediate product and release of symmetrical ketones. Final decomposition to La2O3 takes place with release of CO2.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Yue, Z. (Intern), Suarez Guevara, M. J. (Intern), Watenphul, A. (Ekstern)
Number of pages: 9
Pages: 1-9
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Thermochimica Acta
Volume: 612
ISSN (Print): 0040-6031
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.683 SNIP 1.17 CiteScore 2.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.706 SNIP 1.125 CiteScore 2.18
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.916 SNIP 1.489 CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.628 SNIP 1.513 CiteScore 2.33
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.75 SNIP 1.424 CiteScore 2.1
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Study of Multi-layer Active Magnetic Regenerators Using Magnetocaloric Materials with First and Second Order Phase Transition

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Poster

Abstract
Source: PublicationPreSubmission
Source-ID: 117942122
Publication: Research - peer-review › Poster – Annual report year: 2015

Study on advanced Ce_{0.5}La_{0.1}O_{2–δ}/Gd_{2}Zr_{2}O_{7} buffer layers architecture towards all chemical solution processed coated conductors

Chemical solution deposition is a versatile technique to deposit functional oxide films with low cost. In this study, this approach was employed to grow multi-layered, second-generation, high-temperature superconductors ("coated conductors") with high superconducting properties. The CeO_{0.9}LaO_{0.1}O_{2}/Gd_{2}Zr_{2}O_{7} buffer layer stack and the 200 nm thick YBa_{2}Cu_{3}O_{7} (YBCO) superconducting layer were sequentially deposited on textured NiW substrates using metal-organic deposition routes. The surface texture of the Gd_{2}Zr_{2}O_{7} barrier layer deteriorates when the film thickness increases to 80 nm, although the global texture retains a sharp biaxial orientation, as determined by conventional X-ray diffraction. We paid particular attention to improving the surface quality in terms of crystallographic orientation and local flatness after...
depositing a Ce0.9La0.1O2 thin film as a cap layer. From a comprehensive analysis of the surface morphology and misorientation maps constructed by electron backscattering diffraction, it is found that these improvements are mainly attributed to: (i) the preferential nucleation of Ce0.9La0.1O2 crystals on the Gd2Zr2O7 grains with desirable orientations; and (ii) the predominant two-dimensional growth of the Ce0.9La0.1O2 crystals in the layer. Moreover, the microstructure and superconducting performance of the YBCO superconducting layer were thoroughly characterized and compared with those of films deposited on single-crystal substrates using the same technique. A promising critical current density of 2.2 MA cm⁻² (77 K, self-field) was achieved on such an all chemical derived configuration, demonstrating the high quality of the buffer layer stack and the feasibility of using all chemical solution routes for the fabrication of low-cost coated conductors.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Shanghai Jiao Tong University, Beijing University of Technology
Authors: Yue, Z. (Intern), Ma, L. (Ekstern), Wu, W. (Ekstern), Suo, H. (Ekstern), Grivel, J. (Intern)
Number of pages: 8
Pages: 13275-13282
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 25
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
Backscattering, Buffer layers, Chemicals, Critical current density (superconductivity), Crystal microstructure, Deposition, High temperature superconductors, Lanthanum, Optical waveguides, Organometallics, Oxide films, Single crystals, Superconducting films, Superconducting materials, Textures, X ray diffraction, Yttrium barium copper oxides, Zirconium, Chemical solution deposition, Chemical solution route, Crystallographic orientations, Electron backscattering diffraction, Metal organic deposition, Single crystal substrates, Superconducting performance, Superconducting properties, Cerium DOIs:
10.1039/c5ta00153f
Source: FindIt
Source-ID: 275298557
Publication: Research - peer-review › Journal article – Annual report year: 2015

Study on Fabrication of Ni-5 at.%W Tapes for Coated Conductors from Cylinder Ingots
Ni-5 at.%W (Ni5W) tapes with a strong cube texture were fabricated using the RABiTS technique and by starting from cylindrical shaped ingots. In contrast to a conventional cuboid-shaped ingot, a cylinder shaped ingot has no anisotropy along the axial direction and the resulting tape will therefore, during heavy cold rolling, be characterized by a lower concentration of stress along the edges of the ingot. It can reduce fabrication costs and increase process efficiency. The fraction of cube texture on the surface of the finally recrystallized tapes was investigated using the EBSD technique. It was observed that the fraction of cube texture within 10° from the ideal {001}〈100〉 orientation was ~98% and the fraction of LAGBs was ~90%. The as-obtained tapes have a strong cube texture also very close to the edge of the tape and they would therefore increase the fraction of applicable material while simplifying the heavy rolling process. Accordingly, it suggests that this fabrication method is a good choice to most small scale research laboratories for achieving long length
Ni5W tapes for coated conductors with an easy way and a higher fraction of applicable material.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Beijing University of Technology
Authors: Ma, L. (Ekstern), Suo, H. L. (Ekstern), Yue, Z. (Intern), Wulff, A. C. (Intern), Liang, Y. R. (Ekstern), Grivel, J. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: IEEE Transactions on Applied Superconductivity
Volume: 25
Issue number: 3
Article number: 7800105
ISSN (Print): 1051-8223
Ratings:
- BFI (2018): BFI-level 1
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.47 SNIP 1.113 CiteScore 0.83
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.431 SNIP 1.171 CiteScore 1.32
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.575 SNIP 1.27 CiteScore 1.11
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.364 SNIP 1.063 CiteScore 1.16
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.468 SNIP 1.073
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.452 SNIP 1.033
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.878 SNIP 0.987
- Scopus rating (2007): SJR 0.611 SNIP 1.104
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 0.731 SNIP 0.935
- Scopus rating (2005): SJR 0.645 SNIP 0.996
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.867 SNIP 0.9
- Scopus rating (2003): SJR 0.494 SNIP 1.045
- Web of Science (2003): Indexed yes
Sulfonated copolyimide membranes derived from a novel diamine monomer with pendant benzimidazole groups for fuel cells

Sulfonated polyimides are among the most interesting proton exchange membrane materials with high proton conductivity and good mechanical characteristics. As a major challenge the hydrolytic instability of the polymer backbone is addressed by introducing basic moieties in the polymer main chain. A series of sulfonated copolyimides (SPI) are prepared via random copolymerization of 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTDA) with a new diamine monomer with pendant benzimidazole groups, 2,2′-bis(4-(1H-benzo[d]imidazol-2-yl)phenoxy)benzidine (BIPOB), and a sulfonated diamine monomer 4,4′-bis(4-aminophenoxy)biphenyl-3,3′-disulfonic acid (BAPBDS) at different diamine molar ratios (BAPBDS/BIPOB, 4/1, 6/1, 9/1 and 12/1). With ion exchange capacities in the range of 1.60-2.24 meq g(-1), transparent and ductile membranes are obtained by solution casting. The incorporation of benzimidazole pendant groups significantly improves the hydrolytic stability as well as the radical oxidative stability of the membranes. In addition, the SPI membranes exhibit high proton conductivities of 0.1 S cm(-1) in the fully hydrated state at 60 degrees C and high elastic modulus and tensile strength. Preliminary fuel cell tests demonstrate the technical feasibility and stability of the materials. (C) 2015 Elsevier B.V. All rights reserved.
Sulfur Poisoning of Ni/stabilized-zirconia Anodes: Effect on Long-Term Durability

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Fundamental Electrochemistry
Authors: Hauch, A. (Intern), Hagen, A. (Intern), Hjelm, J. (Intern), Ramos, T. (Intern)
Number of pages: 17
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Tailoring of porosity of yttria-stabilized zirconia tubes as supports for oxygen separation membranes

Pure oxygen gas supplied by ceramic oxygen transport membranes can facilitate reduced CO2 emissions through more efficient gasification processes and CO2 capture and storage. Tubular membranes have some advantages compared to planar membranes, such as better resistance to thermal gradients and more straightforward sealing. The active oxygen separation layer in the membrane should be as thin as possible and therefore supported on a highly porous tubular substrate. In this work tubular porous supports of yttria-stabilized zirconia have been manufactured using thermoplastic extrusion. Two types of poreformers (spherical graphite (d50 18 μm) and polymethyl methacrylate (d50 10 μm)) have been used to form connected macropores, since their spherical geometry limits preferential orientation during extrusion. Their difference in decomposition temperatures also allows a high volume fraction of pore formers without deformation during debinding. The influence of the amount of pore formers (relative to the amount of ceramic and thermoplastics) on the microstructure of sintered samples, as well as the extrudability and ease of debinding of the feedstock, has been studied. Ceramics with 1-20 μm pores, open porosities exceeding 55 % and gas permeabilities close to 10-14 m2 could be produced, demonstrating that thermoplastic extrusion is suitable for fabrication of porous and permeable tubes.

Temperature Dependence and Magnetic Properties of Injection Molding Tool Materials Used in Induction Heating

To analyze the heating phase of an induction heated injection molding tool precisely, the temperature-dependent magnetic properties, B–H curves, and the hysteresis loss are necessary for the molding tool materials. Hence, injection molding tool steels, core materials among other materials have, in this paper, been characterized for their temperature-dependent magnetic properties. The properties have been measured using a vibrating sample magnetometer, able to reach to 350 °C. The established material database comprises the B–H loops, from which the mean B–H curve, relative permeability versus magnetic flux density, and hysteresis loss versus magnetic flux density have been extracted and are presented.
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Magnetics
Volume: 51
Issue number: 9
Article number: 6000507
ISSN (Print): 0018-9464
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.48 SNIP 0.915 CiteScore 1.47
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.565 SNIP 1.207 CiteScore 1.77
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.715 SNIP 1.491 CiteScore 1.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.608 SNIP 1.424 CiteScore 1.75
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.788 SNIP 1.574 CiteScore 1.89
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.829 SNIP 1.445 CiteScore 1.69
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.698 SNIP 1.134
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.644 SNIP 1.098
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.788 SNIP 1.165
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.71 SNIP 1.152
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.913 SNIP 1.232
Scopus rating (2005): SJR 1.024 SNIP 1.258
Scopus rating (2004): SJR 0.813 SNIP 1.129
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.056 SNIP 1.094
Scopus rating (2002): SJR 1.078 SNIP 1.027
Scopus rating (2001): SJR 0.707 SNIP 1.007
Scopus rating (2000): SJR 0.831 SNIP 1.022
Scopus rating (1999): SJR 0.918 SNIP 1.249
Original language: English
Hysteresis loss, Induction heating, Injection molding tool materials, Temperature dependence of magnetic properties
DOIs:
10.1109/TMAG.2015.2428215
Tetrazole substituted polymers for high temperature polymer electrolyte fuel cells

While tetrazole (TZ) has much lower basicity than imidazole and may not be fully protonated in the presence of phosphoric acid (PA), DFT calculations suggest that the basicity of TZ groups can be increased by the introduction of a 2,6-dioxo-phenyl-group in position 5 of TZ. This structure allows hydrogen bonds between TZ protons and ether oxygen atoms, and thereby establishes a resonance stabilised, co-planar structure for tetrazolium ions. Molecular electrostatic potential (MEP) calculations also indicate that tetrazolium ions possess two sites for proton hopping. This makes such materials interesting for use in a high temperature fuel cell (HT PEMFC). Based on these findings, two polymers incorporating the proposed TZ groups were synthesised, formed into membranes, doped with PA and tested for fuel cell relevant properties. At room temperature, TZ-PREEN and commercial meta-PBI showed an equilibrium uptake of 0.5 and 4.7 mol PA per mol heterocycle, respectively, indicating that PBI has higher affinity for PA than TZ-PEEN. The highest achieved PA uptake was ca. 110 wt%, resulting in a proton conductivity of 25 mS cm$^{-1}$ at 160 °C with a low activation energy of about 35 kJ mol$^{-1}$. In a first HT PEMFC test at 160 °C, a peak power density of 287 mW cm$^{-2}$ was achieved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Korea Institute of Science and Technology, Jagiellonian University, Korea University
Authors: Henkensmeier, D. (Ekstern), My Hanh Duong, N. (Ekstern), Brela, M. (Ekstern), Dyduch, K. (Ekstern), Michalak, A. (Ekstern), Jankova Atanasova, K. (Intern), Cho, H. (Ekstern), Hyun Jang, J. (Ekstern), Kim, H. (Ekstern), Cleemann, L. N. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: 14389-14400
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 27
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
DOIs: 10.1039/c5ta01936b

The Critical Choice of PEDOT: PSS Additives for Long Term Stability of Roll-to-Roll Processed OPVs

The impact of additives mixed with poly(3,4-ethylenedioxythiophene):polystyrenesulfonate (PEDOT:PSS) on the stability of organic photovoltaic modules is investigated for fully ambient roll-to-roll (R2R) processed indium tin oxide free modules. Four different PEDOT:PSS inks from two different suppliers are used. The modules are manufactured directly on barrier foil without a UV filter to accelerate degradation and enable completion of the study in a reasonable time span. The modules are subjected to stability testing following well-established protocols developed by the international summit on organic photovoltaic stability (ISOS). For the harsh indoor test (ISOS-L-3) only a slight difference in stability is observed between the different modules. During both ISOS-L-3 and ISOS-D-3 one new failure mode is observed as a result of tiny air inclusions in the barrier foil and a R2R method is developed to detect and quantify these. During outdoor operation (ISOS-O-1) the use of ethylene glycol (EG) as an additive is found to drastically increase the operational stability of the
modules as compared to dimethylsulfoxide (DMSO) and a new failure mode specific to modules with DMSO as the additive is identified. The data are extended in an ongoing experiment where DMSO is used as additive for long-term outdoor testing in a solar park.

The effect of hydrogen pressure on the tolerance for co of high temperature PEM fuel cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Fernandez, S. M. (Intern), Vassiliev, A. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Annual Meeting of the Danish Electrochemical Society 2015, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation
Source: PublicationPreSubmission
Source-ID: 127806532
Publication: Research › peer-review › Conference abstract for conference – Annual report year: 2016
The effect of mesomorphology upon the performance of nanoparticulate organic photovoltaic devices

Scanning transmission X-ray microscopy (STXM) compositional mapping has been used to probe the mesomorphology of nanoparticles (NPs) synthesized from two very different polymer:fullerene blends: poly(3-hexylthiophene) (P3HT): phenyl-C61-butyric acid methyl ester (PCBM) and poly[4,8-bis(2-ethylhexyloxy)benzo(1,2-b:4,5-b')dithiophene-alt-5, 6-bis(octyloxy)-4,7-di(thiophen-2-yl)-(2,1,3-benzothiadiazole)-5,5'-diyl] (PSBTBT): PCBM. The STXM data shows that both blends form core-shell NP structures with similar shell compositions, but with different polymer:fullerene ratios in the core regions. P3HT:PCBM and PSBTBT:PCBM NP organic photovoltaic (OPV) devices have been fabricated and exhibit similar device efficiencies, despite the PSBTBT being a much higher performing low band gap material. By comparing the measured NP shell and core compositions with the optimized bulk hetero-junction (BHJ) compositions, we show that the relatively higher performance of the P3HT:PCBM NP device arises from the fact that its shell composition is much closer to the optimal BHJ value than that of the PSBTBT:PCBM NP device. [All rights reserved Elsevier].

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Newcastle, Lawrence Berkeley National Laboratory
Number of pages: 7
Pages: 102-108
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Solar Energy Materials and Solar Cells
Volume: 138
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.587 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.869 SNIP 1.896 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.204 SNIP 2.396 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.174 SNIP 2.582 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.435 SNIP 2.707 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.175 SNIP 2.638 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.524 SNIP 2.121
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
The effect of microstructure on lattice thermal conductivity of ScN thin films

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Linköping University
Authors: Kerdsongpanya, S. (Ekstern), Hellman, O. (Ekstern), Sun, B. (Ekstern), Koh, Y. K. (Ekstern), Van Nong, N. (Intern), Lu, J. (Ekstern), Simak, S. I. (Ekstern), Alling, B. (Ekstern), Eklund, P. (Ekstern)
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 18B.6
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
ITC2015_Book_of_Abstract_02.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

The effect of molecular geometry on the photovoltaic property of diketopyrrolopyrrole based non-fullerene acceptors

The non-fullerene acceptors with different geometric structures have great impact on light absorption, exciton dissociation, and charge transportation in the active layer of organic solar cells (OSCs). In this paper, we designed and synthesized two diketopyrrolopyrrole based non-fullerene acceptors, Ph(DPP)2 and PhDMe(DPP)2 with similar chemical components but different molecular geometries. Due to its more twisted molecular conformation, PhDMe(DPP)2 shows more blue-shifted absorption bands, higher electron mobility, and better miscibility with the polymer donor poly(3-hexylthiophene) (P3HT) while compared to Ph(DPP)2. Therefore, the resulting P3HT:PhDMe(DPP)2 based OSCs shows a better power conversion efficiency (PCE) of 0.65%, higher than that from P3HT:Ph(DPP)2 based OSCs (0.48%), which can be ascribed to more efficient exciton dissociation and electron transportation in the active layer of P3HT:PhDMe(DPP)2.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Zhejiang University, Aalborg University
The effect of preparation method on the proton conductivity of indium doped tin pyrophosphates

Indium doped tin pyrophosphates were prepared by three synthetic routes. A heterogeneous synthesis from metal oxides with excess phosphoric acid produces crystalline phosphate particles with a phosphorus rich amorphous phase along the grain boundaries. The amorphous phase prevents the agglomeration of particles, hydrolyzes in moist atmosphere as revealed by FT-IR and solid state NMR, and facilitates a high proton conductivity (above $2.5 \times 10^{-2} \text{ S cm}^{-1}$) with high stability at above 120 °C under a water partial pressure of 0.15 atm. This phase can be removed by washing with water, resulting in a dramatic decrease in conductivity as well as significant agglomeration of the particles, as evident in TEM and from particle size distribution measurements. Homogeneous synthesis with soluble metal acetates or chlorides as precursors results in a single crystalline phase with a small particle size, but strongly agglomerated, and a low conductivity at $10^{-7} - 10^{-6} \text{ S cm}^{-1}$ level. Further impregnation of the agglomerates with phosphoric acid does not lead to formation of the phosphorus rich amorphous layers on the surface of the crystals. An intermediate conductivity of $10^{-3} \text{ S cm}^{-1}$ was observed for the acid treated phosphates from the chloride synthesis but no improvement for the acid treated phosphates from the acetate synthesis was observed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Applied Electrochemistry, University of Southern Denmark, Technical University of Denmark
Authors: Anfimova, T. (Intern), Lie-Andersen, T. (Ekstern), Jensen, E. P. (Ekstern), Prag, C. B. (Intern), Nielsen, U. (Ekstern), Sørensen, D. (Ekstern), Skou, E. (Ekstern), Christensen, E. (Intern), Bjerrum, N. J. (Intern), Li, Q. (Intern)
Number of pages: 8
Pages: 209-216
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 278
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.751 SNIP 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.819 SNIP 1.033 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.304 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.902 SNIP 1.274 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.055 SNIP 1.258 CiteScore 2.31
The efficiency and the demagnetization field of a general Halbach cylinder

The maximum magnetic efficiency of a general multipole Halbach cylinder of order $p$ is found as function of $p$. The efficiency is shown to decrease for increasing absolute value of $p$. The optimal ratio between the inner and outer radius, i.e. the ratio resulting in the most efficient design, is also found as function of $p$ and is shown to tend towards smaller and smaller magnet sizes. Finally, the demagnetizing field in a general $p$-Halbach cylinder is calculated, and it is shown that demagnetization is largest either at $\cos 2p\varphi = 1$ or $\cos 2p\varphi = -1$. For the common case of a $p=1$ Halbach cylinder the maximum values of the demagnetizing field are either at $\varphi = 0, \pi$ at the outer radius, where the field is always equal to the remanence, or at $\varphi = \pm \pi/2$ at the inner radius, where it is the magnitude of the field in the bore. Thus to avoid demagnetization the coercivity of the magnets must be larger than these values.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
The Elastocaloric Effect: A Way to Cool Efficiently

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Composites and Materials Mechanics, Universitat de Barcelona
Authors: Tusek, J. (Intern), Engelbrecht, K. (Intern), Millán-Solsona, R. (Ekstern), Mañosa, L. (Ekstern), Vives, E. (Ekstern), Mikkelsen, L. P. (Intern), Pryds, N. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 5
Article number: 1500361
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.124 SNIP 2.045
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.254 SNIP 2.531 CiteScore 14.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.706 SNIP 2.975 CiteScore 15.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.979 SNIP 2.936 CiteScore 13.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.571 SNIP 2.216 CiteScore 9.64
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Original language: English
DOIs:
10.1002/aenm.201500361
The Focused Ion Beam – Scanning Electron Microscope: A tool for sample preparation, two and three dimensional imaging

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bowen, J. R. (Intern)
Number of pages: 80
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
2014_IMAGINE_FIB_SEM_JR_Bowen.pdf

Relations
Activities:
DTU Energy Conversion 2nd International PhD Summer School
Publication: Research › Sound/Visual production (digital) – Annual report year: 2015

The influence of hysteresis on the determination of the magnetocaloric effect in Gd$_2$Si$_2$Ge$_2$

We present a non-equilibrium Preisach-type hysteresis model based on the first order magnetocaloric material Gd$_2$Si$_2$Ge$_2$. The model is developed from isofield magnetization measurements and first order reversal curves, both of which constitute a new and detailed approach to characterizing and modelling magnetocaloric materials. It is shown that the model reproduces the magnetization data, directly measured adiabatic temperature changes and provides a good description of the material behavior under application conditions. We find that the material settles in an area of metastability under continuous magnetization cycles, which effectively limits the adiabatic temperature change by the amount of thermal hysteresis present. We suggest a straightforward method for realistic estimation of the magnetocaloric effect from indirect measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: von Moos, L. (Intern), Bahl, C. (Intern), Nielsen, K. K. (Intern), Engelbrecht, K. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Volume: 48
Issue number: 2
Article number: 025005
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.645 SNIP 0.917
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.693 SNIP 1.046 CiteScore 2.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.069 SNIP 1.383 CiteScore 2.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
The NanoCaTe Project: Nano-carbons for versatile power supply modules

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Fraunhofer Institut für Werkstoff- und Strahltechnik, LEITAT Technological Center, VTT - Technical Research Centre of Finland, INVENT GmbH, Quick-Ohm Küpper & Co. GmbH, KIM Knowledge innovation market, Infineon Technologies Austria AG, Alpcon, Technische Universität Graz, Dresden University of Technology, Aalborg University
Theoretical understanding about the interaction between iron carbide and graphitic layers towards oxygen reduction

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Hu, Y. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Zhong, L. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Conference on Electrochemical Science and Technology 2015, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences

**Bibliographical note**
Oral by Yang Hu
Source: PublicationPreSubmission
Source-ID: 127806554
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

The performance of a combined solar photovoltaic (PV) and thermoelectric generator (TEG) system

The performance of a combined solar photovoltaic (PV) and thermoelectric generator (TEG) system is examined using an analytical model for four different types of commercial PVs and a commercial bismuth telluride TEG. The TEG is applied directly on the back of the PV, so that the two devices have the same temperature. The PVs considered are crystalline Si (c-Si), amorphous Si (a-Si), copper indium gallium (di) selenide (CIGS) and cadmium telluride (CdTe) cells. The degradation of PV performance with temperature is shown to dominate the increase in power produced by the TEG, due to the low efficiency of the TEG. For c-Si, CIGS and CdTe PV cells the combined system produces a lower power and has a lower efficiency than the PV alone, whereas for an a-Si cell the total system performance may be slightly increased by the TEG.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern)
Pages: 187–194
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Solar Energy
Volume: 120
ISSN (Print): 0038-092X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.52 SJR 1.547 SNIP 1.748
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Thermal decomposition of barium valerate in argon

The thermal decomposition of barium valerate ($\text{Ba(C}_4\text{H}_9\text{CO}_2\text{)}(\text{2})$/$\text{Ba-pentanoate}$) was studied in argon by means of thermogravimetry, differential thermal analysis, IR-spectroscopy, X-ray diffraction and hot-stage optical microscopy. Melting takes place in two different steps, at 200 degrees C and 280 degrees C and evidence was found for the solidification of the melt at 380-440 degrees C, i.e. simultaneously with the onset of decomposition. Between 400 degrees C and 520 degrees C ($\text{Ba(C}_4\text{H}_9\text{CO}_2\text{)}(\text{2})$ decomposes in two main steps, first into $\text{BaCO}_3$ with release of $\text{C}_4\text{H}_9\text{COC}_4\text{H}_9$ ($5$-nonanone), whereas final conversion to $\text{BaO}$ takes place with release of $\text{CO}_2$. Elemental carbon that is left as a by-product is finally slowly burned by the residual oxygen present in the Ar atmosphere. (C) 2015 Elsevier B.V. All rights reserved.
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Electrofunctional materials, Universidad Autonoma de Barcelona
Authors: Torres, P. (Ekstern), Norby, P. (Intern), Grivel, J. (Intern)
Pages: 120-128
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Analytical and Applied Pyrolysis
Volume: 116
ISSN (Print): 0165-2370
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.11 SJR 1.353 SNIP 1.533
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.497 SNIP 1.63 CiteScore 4.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.714 SNIP 1.967 CiteScore 4.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.046 SNIP 1.948 CiteScore 3.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.439 SNIP 1.792 CiteScore 3.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.415 SNIP 1.556 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.191 SNIP 1.427
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.262 SNIP 1.407
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.264 SNIP 1.458
Scopus rating (2007): SJR 1.368 SNIP 1.946
Scopus rating (2006): SJR 0.881 SNIP 1.413
Scopus rating (2005): SJR 0.786 SNIP 1.243
Scopus rating (2004): SJR 1.099 SNIP 1.242
Scopus rating (2003): SJR 0.811 SNIP 1.369
Scopus rating (2002): SJR 1.281 SNIP 1.205
Scopus rating (2001): SJR 1.319 SNIP 1.542
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.004 SNIP 1.141
Scopus rating (1999): SJR 0.807 SNIP 1.161
Original language: English
Barium valerate, Thermal decomposition, TG/DTA, FTIR, X-ray powder diffraction
DOIs:
10.1016/j.jaap.2015.09.018
Thermal decomposition of yttrium(III) hexanoate in argon

The thermal decomposition of yttrium(III) hexanoate (Y(C5H11CO2)3)·xH2O in argon was studied by means of thermogravimetry, differential thermal analysis, IR-spectroscopy, X-ray diffraction at a laboratory Cu-tube source and in-situ experiments at a synchrotron radiation source as well as hot-stage optical microscopy. Dehydration occurs between 40°C and 110°C and is accompanied by a transition from solid to liquid crystalline state. At the onset of the main decomposition stage of the anhydrous Y(C5H11CO2)3, solidification takes place in the 315-335°C range. Y(C5H11CO2)3 decomposes in a single step into Y2O2CO3 with release of CO2 and 6-undecanone between 280°C and 490°C. A side reaction appears to yield elemental carbon and volatile decane (C10H22). Y2O2CO3 is converted to Y2O3 with release of CO2 between 500°C and 975°C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, University of Hamburg
Authors: Grivel, J. (Intern), Suarez Guevara, M. J. (Intern), Attique, F. (Intern), Zhao, Y. (Ekstern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Watenphul, A. (Ekstern), Zimmermann, M. (Ekstern)
Pages: 237–243
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Analytical and Applied Pyrolysis
Volume: 112
ISSN (Print): 0165-2370
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.11 SJR 1.353 SNIP 1.533
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.497 SNIP 1.63 CiteScore 4.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.714 SNIP 1.967 CiteScore 4.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.046 SNIP 1.948 CiteScore 3.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.439 SNIP 1.792 CiteScore 3.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.415 SNIP 1.556 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.191 SNIP 1.427
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.262 SNIP 1.407
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.264 SNIP 1.458
Thermoelastic and structural properties of ionically conducting cerate perovskites: (II) SrCeO₃ between 1273 K and 1723 K

The temperature dependence of the crystal structure and the thermoelastic properties of SrCeO₃ have been determined from Rietveld refinement of high resolution, neutron time-of-flight powder diffraction data collected in 5 K intervals between 1273 K and 1723 K. No evidence was found for critical behaviour in the amplitudes of the modes that soften in zone boundary phase transitions in perovskite-structured phases suggesting SrCeO₃ may remain orthorhombic, space group Pbnm from 1.2 K up to the 1 atm melting point of 2266 K. The temperature variation of the crystal structure has been determined from mode decomposition techniques and the structural evolution has been inferred from the temperature-dependences of the spontaneous shear strain and the order parameter associated with the anti-phase tilt. Thermoelastic properties have been derived from the temperature variation of the unit cell, isobaric heat capacity, and atomic displacement parameters and shows good agreement with earlier work carried out on the lightly doped system SrCe0.95Yb0.05Oᵢ (ᵢ [similar] 3). Temperature-dependent corrections for the bond valence parameters for strontium and cerium are reported.
The role of sacrificial fugitives in thermoplastic extrusion feedstocks on properties of MgO supports for oxygen transport membranes

2014AbstractThree different compositions of MgO compounds were investigated for use in oxygen transport membranes. Porous MgO supports were extruded using different kind (size, morphology and chemistry) of pore formers: A flaky graphite, a spherical graphite and ideal spheres of PMMA. The influence of the pore former on microstructure, gas permeation and the mechanical properties for various sintering temperatures were investigated. The gas permeation behavior of the MgO supports was highly dependent on pore neck size and total open porosity. MgO substrate, with 20% spherical graphite as a pore former, sintered at 1300°C for 2 h, showed a total porosity of 42.5% and gas permeability of
4.7 × 10⁻¹⁶m². Subsequently, the 4-point bending strengths of this substrate, scaled to an effective volume of 10 mm³, were 77 and 60 MPa for room and operation temperature (850°C). Both, permeation rate and mechanical strength is sufficient for using the support for further investigations in OTM. © 2014 Elsevier Ltd. All rights reserved.
The Solar Textile Challenge: How It Will Not Work and Where It Might

Solar textiles are highlighted as a future technology with transformative power within the fields of both textiles and solar cells provided that developments are made in critical areas. Specifically, these are fundamental solutions to materials and material combinations with mechanical stability and flexibility imposed by textile architectures, scientific solutions to achieve high carrier transport efficiency and optical transmission in a textile topology, technical solutions to controlling the physical disposition of the anode and cathode along with their specific and error-free contacting and, finally, practical solutions to fast and efficient manufacture and integration. The areas of application and the penetration of solar textiles into our everyday life are expected to be explosive pending efficient developments within these four key areas. A shortcoming in one or more of these will, however, lead to the solar textiles being banned to academic existence.
Scopus rating (2012): SJR 3.046 SNIP 1.563 CiteScore 6.72
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.945 SNIP 1.134
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.973 SNIP 0.72
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.291 SNIP 0.48
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.273 SNIP 0.495
Scopus rating (2006): SJR 0.243 SNIP 0.372
Scopus rating (2005): SJR 0.195 SNIP 0.285
Scopus rating (2004): SJR 0.214 SNIP 0.276
Scopus rating (2003): SJR 0.276 SNIP 0.419
Scopus rating (2002): SJR 0.312 SNIP 0.586
Scopus rating (2001): SJR 0.292 SNIP 0.496
Scopus rating (2000): SJR 0.422 SNIP 0.556
Scopus rating (1999): SJR 0.511 SNIP 0.708
Original language: English
DOIs: 10.1002/cssc.201403377
Source: PublicationPreSubmission
Source-ID: 105673011
Publication: Research - peer-review › Journal article – Annual report year: 2015

The stability of poly(2,2′-(m-phenylene)-5,5′-bibenzimidazole) membranes in aqueous potassium hydroxide
In the form of membranes, poly(2,2′-(m-phenylene)-5,5′-bibenzimidazole) (mPBI) is known to exhibit high ionic conductivity when doped with aqueous KOH, which makes it interesting as electrolyte in e.g. alkaline fuel cells and water electrolyzers. The conductivity peaks at KOH concentrations around 25wt%. This work is devoted to a comprehensive stability study of mPBI in aqueous KOH of different concentrations for up to 200 days under conditions relevant for electrochemical energy conversion technologies. The polymer membranes were kept at 88°C in aqueous KOH with concentrations ranging from 0 to 50wt%, and the chemical and physicochemical changes were monitored. The degradation was connected to the hydrolysis of the polymer backbone and the degradation rate increased with increasing KOH concentration. In the lower concentration range mPBI proved to be stable but exhibited low ionic conductivity (10⁻⁴S/cm⁻¹). The preparation of a porous mPBI matrix was demonstrated as an effective approach to increase the ionic conductivity in the lower KOH concentration range, with great potential for further improvement through optimization of the porous structure.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Jankova Atanasova, K. (Intern), Li, Q. (Intern), Bjerrum, N. J. (Intern), Jensen, J. O. (Intern)
Number of pages: 8
Pages: 422-429
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 492
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
The Total Lifetime Cost of a Magnetic Refrigerator

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
The universal influence of contact resistance on TEG efficiency

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. International Conference on Thermoelectrics (ICT) 2015
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
The_universal_influence.pdf
Source: PublicationPreSubmission
Source-ID: 118916309
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

The Universal Influence of Contact Resistance on the Efficiency of a Thermoelectric Generator
The influence of electrical and thermal contact resistance on the efficiency of a segmented thermoelectric generator is investigated. We consider 12 different segmented p-legs and 12 different segmented n-legs, using eight different p-type and eight different n-type thermoelectric materials. For all systems, a universal influence of both the electrical and thermal contact resistance is observed on the leg’s efficiency, when the systems are analyzed in terms of the contribution of the contact resistance to the total resistance of the leg. The results are compared with the analytical model of Min and Rowe. In order for the efficiency not to decrease by more than 20%, the contact electrical resistance should be less than 30% of the total leg resistance for zero thermal contact resistance, while the thermal contact resistance should be less than 20% for zero electrical contact resistance. The universal behavior also allowed the maximum tolerable contact resistance for a segmented system to be found, i.e., the resistance at which a leg of only the high-temperature thermoelectric material has the same efficiency as the segmented leg with a contact resistance at the interface. If, e.g., segmentation increases the efficiency by 30%, then an electrical contact resistance of 30% or a thermal contact resistance of 20% can be tolerated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern)
Number of pages: 8
Pages: 2869-2876
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Electronic Materials
Volume: 44
Issue number: 8
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Thin films of CZTS prepared by Pulsed Laser Deposition

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials, Experimental Surface and Nanomaterials Physics
Authors: Cazzaniga, A. C. (Intern), Ettlinger, R. B. (Intern), Engberg, S. L. J. (Intern), Canulescu, S. (Intern), Crovetto, A. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern)

Electronic versions:
The_universal_influence_postprint.pdf
DOIs: 10.1007/s11664-015-3731-7
Source: FindIt
Source-ID: 275326561
Publication: Research - peer-review › Journal article – Annual report year: 2015
Thiophene in Conducting Polymers: Synthesis of Poly(thiophene)s and Other Conjugated Polymers Containing Thiophenes, for Application in Polymer Solar Cells

Conducting polymers based on thiophene are described. The polymers include poly(thiophene) with and without side-chains and other conjugated polymers in general, based on thiophene. The synthesis and characteristics of the polymers are described along with the application of these as light-absorbing materials in polymer solar cells.

Three dimensional corrugated organic photovoltaics for building integration; improving the efficiency, oblique angle and diffuse performance of solar cells

The lamination of OPV modules to corrugated roof cladding has been undertaken. The 3-dimensional form of the cladding provides three advantages for outdoor OPV deployment; firstly the ‘footprint’ of the solar cell is reduced, which leads to B10% improved power conversion (PCE) efficiency per unit area. Secondly, the oblique angle performance is enhanced, leading to increased output in the early morning and evening. Indoor characterisation showed a 9-fold enhancement in efficiency was obtainable, when compared to a flat module. Thirdly, an improvement in performance under diffuse lighting conditions was measured, when compared to a flat module. The average daily yield of the 3D module was 17–29% higher than a flat module, with higher relative enhancements observed on cloudier days. Geographically, the 3D module appears to be well-suited to countries with a high latitude, due to the enhanced diffuse light levels and the fact that tilting the module in both ‘latitude’ and ‘longitude’ directions away from normal, leads to the best achievable enhancement in solar cell performance. The approach set out in this paper could yield a product that has profound advantages over existing BIPV products and is potentially applicable to other flexible inorganic solar cell technologies.
Three-Dimensional Modeling of Glass Lens Molding

The required accuracy for the final dimensions of the molded lenses in wafer-based precision glass molding as well as the need for elimination of costly experimental trial and error calls for numerical simulations. This study deals with 3D thermo-mechanical modeling of the wafer-based precision glass lens molding process. First, a comprehensive 3D thermo-mechanical model of glass is implemented into a FORTRAN user subroutine (UMAT) in the FE program ABAQUS, and the developed FE model is validated with both a well-known sandwich seal test and experimental results of precision molding of several glass rings. Afterward, 3D thermo-mechanical modeling of the wafer-based glass lens manufacturing is performed to suggest a proper molding program (i.e., the proper set of process parameters including preset force-time and temperature-time histories) for molding a wafer to a desired dimension and quality. Moreover, the effect of some important process parameters such as cooling rate and pressing temperature on the final size and residual stress inside the wafer is
evaluated. Finally, it is noted that the suggested molding program minimizes the costly empirical efforts and raises the process efficiency.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Manufacturing Engineering
Authors: Sarhadi, A. (Intern), Hattel, J. H. (Intern), Hansen, H. N. (Intern)
Pages: 182–195
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Applied Glass Science
Volume: 6
Issue number: 2
ISSN (Print): 2041-1286
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.632 SNIP 1.052 CiteScore 1.9
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.605 SNIP 0.995 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.854 SNIP 1.27 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.788 SNIP 1.824 CiteScore 2.27
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.785 SNIP 1.819 CiteScore 1.73
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.646 SNIP 1.574
ISI indexed (2011): ISI indexed no
Original language: English
DOIs: 10.1111/ijag.12110
Source: PublicationPreSubmission
Source-ID: 105176492
Publication: Research - peer-review » Journal article – Annual report year: 2015

**Tin- and Lead-Based Perovskite Solar Cells under Scrutiny: An Environmental Perspective**
The effect of substituting lead with tin in perovskite-based solar cells (PSCs) has shows that lead is preferred over tin by a lower cumulative energy demand. The results, which also include end-of-life management, show that a recycling scenario that carefully handles emission of lead enables use of lead in PSCs with little environmental impact. All other scenarios result in catastrophic emission of lead to the environment that would spell an end to widespread use of lead in PSCs.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technical University of Cartagena, Universidad Politecnica de Cartagena
Authors: Serrano-Luján, L. (Ekstern), Espinosa Martinez, N. (Intern), Larsen-Olsen, T. T. (Intern), Abad, J. (Ekstern), Urbina, A. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences
Topology Optimization of an Actively Cooled Electronics Section for Downhole Tools

Active cooling systems represent a possible solution to the electronics overheating that occurs in wireline downhole tools operating in high temperature oil and gas wells. A Peltier cooler was chosen to maintain the downhole electronics to a tolerable temperature, but its integration into the downhole electronics unit proved to be challenging, because of the space constraints and the proximity of the cooling zone (electronics) to the heat sink (well fluid). The topology optimization approach was therefore chosen to optimize the thermal design of the actively cooled electronics section and the SIMP (Solid Isotropic Material with Penalization) method was implemented in COMSOL Multiphysics. Several optimized designs were obtained for different operating conditions and their sensitivity to the change in the boundary conditions was evaluated. A final design for the electronics unit was selected, according to the topology optimization results and assembly constraints, and compared to the optimized cases.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Soprani, S. (Intern), Klaas Haertel, J. H. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern), Engelbrecht, K. (Intern)
Number of pages: 7
Publication date: 2015

Host publication information
Title of host publication: Proceedings. COMSOL Conference 2015
Publisher: COMSOL Inc.
Main Research Area: Technical/natural sciences
Conference: COMSOL Conference 2015, Grenoble, Switzerland, 14/10/2015 - 14/10/2015
Topology optimization, SIMP, Electronics cooling
Electronic versions:
Topology Optimization of Thermal Heat Sinks

In this paper, topology optimization is applied to optimize the cooling performance of thermal heat sinks. The coupled two-dimensional thermofluid model of a heat sink cooled with forced convection and a density-based topology optimization including density filtering and projection are implemented in COMSOL Multiphysics. The optimization objective is to minimize the heat sink's temperature for a prescribed pressure drop and fixed heat generation. To conduct the optimization, COMSOL's Optimization Module with GCMMA as the optimization method is used. The implementation of this topology optimization approach in COMSOL Multiphysics is described in this paper and results for optimized two-dimensional heat sinks are presented. Furthermore, parameter studies regarding the effect of the prescribed pressure drop of the system on Reynolds number and realized heat sink temperature are presented and discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Klaas Haertel, J. H. (Intern), Engelbrecht, K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern)
Number of pages: 6
Publication date: 2015

Host publication information
Title of host publication: Proceedings. COMSOL conference 2015
Main Research Area: Technical/natural sciences
Conference: COMSOL Conference 2015, Grenoble, Switzerland, 14/10/2015 - 14/10/2015

Relations
Projects:
Topology Optimization of Thermal Heat Sinks

Transition metal carbides (WC, Mo₂C, TaC, NbC) as potential electrocatalysts for the hydrogen evolution reaction (HER) at medium temperatures

One limitation for large scale water electrolysis is the high price of the Pt cathode catalyst. Transition metal carbides, which are considered as some of the most promising non-Pt catalysts, are less active than Pt at room temperature. The present work demonstrates that the situation is different at medium temperatures (200-400 degrees C). By introducing a new setup which makes use of molten KH₂PO₄ as electrolyte, a model system for solid acid membrane electrolyser cells was obtained. Metal carbide coated wires prepared by a two-step oxidation carburization reaction of the metal wire surfaces were used as electrodes and allowed the measurement of the intrinsic catalytic properties of different transition metal carbides in direct comparison to Pt at 260 degrees C. Under these conditions, the activity in the hydrogen evolution reaction (HER) followed the order WC > Pt approximate to MO₂C > NbC > TaC. Copyright (C) 2014, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technische Universität München
Authors: Meyer, S. (Ekstern), Nikiforov, A. V. (Intern), Petrushina, I. M. (Intern), Köhler, K. (Ekstern), Christensen, E. (Intern), Jensen, J. O. (Intern), Bjerrum, N. J. (Intern)
Pages: 2905-2911
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Volume: 40
Issue number: 7
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Original language: English

CHEMISTRY, ELECTROCHEMISTRY, ENERGY, TUNGSTEN-CARBIDE, MOLYBDENUM BORIDE, OXIDE SURFACES, WATER, ELECTROLYSIS, CATALYSTS, PLATINUM, OXIDATION, BEHAVIOR, AMMONIA, Medium temperature water electrolysis, Hydrogen evolution reaction (HER), Molten potassium dihydrogen phosphate, Non-platinum electrocatalyst

DOIs:
10.1016/j.ijhydene.2014.12.076

Source: Findit
Source-ID: 274390537
Publication: Research - peer-review › Journal article – Annual report year: 2015
Trends in energy supply integration: Solar PV

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Lauritzen, H. (Intern)
Pages: 56-58
Publication date: 2015

Host publication information
Title of host publication: DTU International Energy Report 2015: Energy systems integration for the transition to non-fossil energy systems
Publisher: Technical University of Denmark (DTU)
Editors: Hvidtfeldt Larsen, H., Sønderberg Petersen, L.
ISBN (Print): 978-87-550-3970-4
Main Research Area: Technical/natural sciences
Electronic versions:
Publication: Research - peer-review › Book chapter – Annual report year: 2015

Trends in energy supply integration: Fuel cells and electrolyzers

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Mogensen, M. B. (Intern), Stephens, I. E. (Intern)
Pages: 67-69
Publication date: 2015

Host publication information
Title of host publication: DTU International Energy Report 2015: Energy systems integration for the transition to non-fossil energy systems
Publisher: Technical University of Denmark (DTU)
Editors: Hvidtfeldt Larsen, H., Sønderberg Petersen, L.
ISBN (Print): 978-87-550-3970-4
Main Research Area: Technical/natural sciences
Electronic versions:
Publication: Research - peer-review › Book chapter – Annual report year: 2015

Trends in energy supply integration: Energy storage

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centro Nacional de Energías Renovables
Authors: Aranguren, R. G. (Ekstern), Pedersen, A. S. (Intern)
Pages: 73-76
Publication date: 2015

Host publication information
Title of host publication: DTU International Energy Report 2015: Energy systems integration for the transition to non-fossil energy systems
Publisher: Technical University of Denmark (DTU)
Editors: Hvidtfeldt Larsen, H., Sønderberg Petersen, L.
ISBN (Print): 978-87-550-3970-4
Main Research Area: Technical/natural sciences
Electronic versions:
Triple phase boundary specific pathway analysis for quantitative characterization of solid oxide cell electrode microstructure

The density and percolation of Triple phase boundary sites are important quantities in analyzing microstructures of solid oxide fuel cell electrodes from tomography data. However, these measures do not provide descriptions of the quality of the TPB sites in terms of the length and radius of the pathways through which they can be reached. New methods for performing TPB specific pathway analysis on 3D image data are introduced, analyzing the pathway properties of each TPB site in the electrode structure. The methods seek to provide additional information beyond whether the TPB sites are percolating or not by also analyzing the pathway length to the TPB sites and the bottleneck radius of the pathway. We show how these methods can be utilized in quantifying and relating the TPB specific results to cell test data of an electrode reduction protocol study for Ni/Scandia-and-Yttria-doped-Zirconia (Ni/ScYSZ) anodes. A study of the TPB density and particle size distribution alone did not provide an explanation for the differences observed in electrode performance. However, the analysis of pathway lengths to the TPBs and the bottleneck radii to reach these TPB sites provided valuable microstructural insight that supported the findings from the electrochemical characterization of the Ni/ScYSZ anodes.
Tunable exchange bias effect in magnetic Bi$_{0.9}$Gd$_{0.1}$Fe$_{0.9}$Ti$_{0.1}$O$_3$ nanoparticles at temperatures up to 250K

The exchange bias (EB) effect has been observed in magnetic Bi$_{0.9}$Gd$_{0.1}$Fe$_{0.9}$Ti$_{0.1}$O$_3$ nanoparticles. The influence of magnetic field cooling on the exchange bias effect has also been investigated. The magnitude of the exchange bias field (HEB) increases with the cooling magnetic field, showing that the strength of the exchange bias effect is tunable by the field cooling. The HEB values are also found to be dependent on the temperature. This magnetically tunable exchange bias obtained at temperatures up to 250K in Bi$_{0.9}$Gd$_{0.1}$Fe$_{0.9}$Ti$_{0.1}$O$_3$ nanoparticles may be worthwhile for potential applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Micro- and Nanotechnology, BioLabChip, Molecular Windows, Bangladesh University of Engineering and Technology, Yamagata University
Authors: Basith, M. A. (Ekstern), Khan, F. A. (Ekstern), Ahmmad, B. (Ekstern), Kubota, S. (Ekstern), Hirose, F. (Ekstern), Ngo, D. (Intern), Hung, T. Q. (Intern), Mølhave, K. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Physics
Volume: 118
Article number: 023901
ISSN (Print): 0021-8979
Ratings:
BFI (2018): BFI-level 1
Two level undercut-profile substrate for filamentary YBa$_2$Cu$_3$O$_7$ coated conductors: Fast Track Communication

A novel substrate design is presented for scalable industrial production of filamentary coated conductors (CCs). The new substrate, called ‘two level undercut-profile substrate (2LUPS)’, has two levels of plateaus connected by walls with an undercut profile. The undercuts are made to produce a shading effect during subsequent deposition of layers, thereby creating gaps in the superconducting layer deposited on the curved walls between the two levels. It is demonstrated that such 2LUPS-based CCs can be produced in a large-scale production system using standard deposition processes, with no additional post-processing. Inspection of the conductor cross-section reveals that the deposited superconducting layer is physically separated at the 2LUPS undercuts. Filament decoupling is also seen in maps of the remanent magnetic field and confirmed by transport measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Wind Energy Systems, Materials science and characterisation, Imaging and Structural Analysis, Department of Physics, Quantum Physics and Information Technology, Slovak Academy of Sciences, Slovak University of Technology, Bruker HTS GmbH, SUBRA IVS
Authors: Wulff, A. C. (Intern), Solovyov, M. (Ekstern), Gömöry, F. (Ekstern), Abrahamsen, A. B. (Intern), Mishin, O. V. (Intern), Usoskin, A. (Ekstern), Rutt, A. (Ekstern), Lundeman, J. (Ekstern), Thydén, K. T. S. (Intern), Hansen, J. O. B. (Ekstern), Grivel, J. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Superconductor Science and Technology
Volume: 28
Issue number: 7
Article number: 072001
ISSN (Print): 0953-2048
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.849 SNIP 1.261 CiteScore 2.07
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.796 SNIP 1.343 CiteScore 2.08
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.054 SNIP 1.178 CiteScore 1.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.873 SNIP 1.144 CiteScore 1.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.243 SNIP 1.089 CiteScore 1.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.403 SNIP 1.352 CiteScore 2.4
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.453 SNIP 1.278
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.266 SNIP 1.426
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.9 SNIP 1.397
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.365 SNIP 1.48
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.409 SNIP 1
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.382 SNIP 1.164
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.118 SNIP 0.993
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.248 SNIP 1.42
Scopus rating (2002): SJR 1.551 SNIP 1.286
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.764 SNIP 1.359
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.811 SNIP 1.178
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.123 SNIP 1.196
Original language: English
Coated conductors, Metal substrate, Filamentary structures, Critical current, Remanent magnetic field
Electronic versions:
Two_level_undercut_profile_substrate_for_filamentary_YBa2Cu3O7_coated_conductors_postprint.pdf. Embargo ended: 12/05/2016
DOIs:
10.1088/0953-2048/28/7/072001
Source: Findit
Source-ID: 274838154
Publication: Research - peer-review › Journal article – Annual report year: 2015

Projects:

Tracking the Microstructure Evolution of an Operating Lithium-Sulphur Battery in Three Dimensions

Department of Energy Conversion and Storage
Imaging and Structural Analysis

Chalmers University of Technology
Period: 16/02/2018 → 17/08/2018
Number of participants: 2
x-ray tomography, battery
Project ID: DTU-034
Number of related Ph.D. students: 0
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
De Angelis, Salvatore (Intern)

Relations
Related projects:
ESS & MAX IV: Cross border science and society
Project

Design and structuring of electrospun nanofiber non-Pt catalysts and electrode for high temperature proton exchange membrane fuel cells
Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student:
Bompolaki, Eftychia (Intern)
Supervisor:
Zhang, Wenjing (Angela) (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

High Resolution X-ray Diffraction Contrast Tomography
Department of Energy Conversion and Storage
Period: 15/11/2017 → 14/11/2020
Number of participants: 3
Phd Student:
Lucas, Mariana Mar (Intern)
Supervisor:
Poulsen, Henning Friis (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Development of a versatile slip-ring/rotary-union based in-operando high temperature functional material test cell for the DanMAX beamline
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Neutrons and X-rays for Materials Physics
Period: 01/10/2017 → 31/03/2018
Number of participants: 3
X-ray synchrotron scattering
Acronym: Op-Stage
Project ID: DTU-029
Number of related Ph.D. students: 1
Project participant:
Karlsson, Maths (Ekstern)
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
Sierra Trujillo, José Xavier (Intern)

Relations
Related projects:
ESS & MAX IV: Cross border science and society
Project

Computational design of electrocatalysts for CO2 reduction
Department of Energy Conversion and Storage
Period: 01/09/2017 → 31/08/2020
Number of participants: 3
Phd Student:
Kildgaard, Jens Vive (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Development of Porous Electrodes for Alkaline Electrolyzers**
Department of Energy Conversion and Storage
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Reumert, Alexander Kappel (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Kraglund, Mikkel Rykær (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

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**In situ Structural Characterization of Multilayer Formation during Large-scale Processing of 3rd Generation Solar Cells**
Department of Energy Conversion and Storage
Period: 01/09/2017 → 26/10/2017
Number of participants: 3
Phd Student:
Rogowska, Melania (Intern)
Supervisor:
Kuhn, Luise Theil (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

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**In-situ Ptychographic Studies of Lithium-Sulphur Micro-Batteries**
PtycoBat exploits a novel battery geometry designed to capitalize on recent gains in high-resolution imaging offered by synchrotron X-ray ptychography. This will be used to explore degradation processes in potential next generation high capacity Li-S battery technology in-situ). It is expected that the kinetics and mechanisms of these processes will be observed for the first time and that the exploratory project will lay the groundwork for future full 3D in-situ imaging at MAXIV.
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Chalmers University of Technology
Period: 15/08/2017 → 15/02/2018
Number of participants: 3
Acronym: PtychoBat
Project ID: DTU-022
Number of related Ph.D. students: 0
Project participant:
Matic, Aleksandar (Ekstern)
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
De Angelis, Salvatore (Intern)

Relations
Related projects:
ESS & MAX IV: Cross border science and society
Project

3D electron microscopy of nanostructures in energy devices
Department of Energy Conversion and Storage
Period: 01/08/2017 → 31/07/2020
Number of participants: 4
Phd Student:
Colding-Jørgensen, Sofie (Intern)
Supervisor:
Schmidt, Søren (Intern)
Simonsen, Søren Bredmose (Intern)
Main Supervisor:
Kuhn, Luise Theil (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Thermochemical Heat Storage
Department of Energy Conversion and Storage
Period: 01/07/2017 → 30/06/2020
Number of participants: 3
Phd Student:
Karabanova, Anastasiiia (Intern)
Supervisor:
Johnsen, Rune E. (Intern)
Main Supervisor:
Blanchard, Didier (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

New Concepts for Efficient Immobilization of Enzymes in Inorganic Membrane Reactors
Department of Energy Conversion and Storage
Period: 01/06/2017 → 31/05/2020
Number of participants: 4
Phd Student:
Lehmann, Jonas (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Pinelo, Manuel (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Nanoscale design of Ammonia Carriers for Air Pollution Control (NANOCONTROL)
Development of materials and multilayer structures for adsorption of ammonia.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/05/2017 → 30/04/2021
Number of participants: 1
gas adsorption, ceramic processing
Acronym: NANOCONTROL
Number of related Ph.D. students: 1
Project participant:
Kaiser, Andreas (Intern)

Commercial project SOFC related
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 01/05/2017 → 30/04/2018
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Nanocrafts - nano jewelry proof of concept
At DTU Nanotech several nanotechnologies were intensively used for texturing, patterning, and protection of surfaces. Nanotechnology can provide a new space for creative design in jewelry with unique features and effects (for instance optical effects implied by nanostructures), bring the deep meaning of emotions and relations to a new level – the nanolevel.
With significant value to the jewelry industry nanotechnology can result in unique technical qualities such as improved durability of items and fraud protection and data encryption technology, and a new way of sensing the item. Micro and nanopatterning allow individual design fabrication on a single wafer. With nanoceramic layers, we can protect golden or other jewelry items from mechanical damage or natural degradation. In this project, we apply
•Surface nanostructuring for physical effects enhancement
•Optical coloring with thin film deposition
•Visual patterning with laser engraving and UV photolithography
•Nanoplasmonic coloring
•Laser engraving on surfaces for data encryption and individual design patterns at the scale of few micrometers

Department of Energy Conversion and Storage
Department of Micro- and Nanotechnology
Silicon Microtechnology
Period: 01/05/2017 → 30/09/2017
Number of participants: 1
Acronym: Nanocrafts
Project participant:
Plakhotnyuk, Maksym (Intern)

GIANT-E: Microstructural forging of electromechanically active bulk ceria
Department of Energy Conversion and Storage
Period: 15/04/2017 → 14/04/2020
Number of participants: 3
Phd Student: 
Kabir, Ahsanul (Intern)
Supervisor: 
Van Nong, Ngo (Intern)
Main Supervisor: 
Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

SOFC stack project II
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/04/2017 → 01/04/2018
Number of participants: 1
Project participant: 
Wulff, Anders Christian (Intern)

Fabrication and electrical properties of advanced thin film materials for resistive switching memories
Department of Energy Conversion and Storage
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
Phd Student: 
Li, Yang (Intern)
Supervisor: 
Esposito, Vincenzo (Intern)
Traulsen, Marie Lund (Intern)
Main Supervisor: 
Pryds, Nini (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Synthesis and characterization of Tubular Oxygen transport membranes
Department of Energy Conversion and Storage
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
Phd Student: 
Martinez Aguilera, Lev (Intern)
Supervisor: 
Bjørnetun Haugen, Astri (Intern)
Kaiser, Andreas (Intern)
Main Supervisor: 
Kiebach, Wolff-Ragnar (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD
Giant-E - Ceria Thin Films Giant Electrostrictors

Department of Energy Conversion and Storage
Period: 15/02/2017 → 14/02/2020
Number of participants: 4
Phd Student: Santucci, Simone (Intern)
Supervisor: Lubomirsky, Igor (Ekstern)
Pryds, Nini (Intern)
Main Supervisor: Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Investigation of metallic-ceramic 3D network-structures for solid oxide fuel cell technology
Investigation of metallic/ceramic Cu-Mn/Cu-Mn-O spinel foam structures and development of Cu-Mn/Cu-Mn-O spinel oxide nanofibers.

Department of Energy Conversion and Storage
Electrofunctional materials
Proton conductors
Mixed Conductors
Period: 01/02/2017 → 23/06/2017
Number of participants: 4
SOFC, oxide spinel, SEM-EDS, microstructure, thermal analysis, electrochemistry, Nanofibers, crystallography
Project participant: Lund, Rasmus Kvist (Ekstern)
Supervisor: Zhang, Wenjing (Angela) (Intern)
Main Supervisor: Wulff, Anders Christian (Intern)

Modelling of ultrafast scattering experiments probing electronic dynamics in solar cells

Department of Energy Conversion and Storage
Project
Period: 15/01/2017 → 14/01/2020
Number of participants: 3
Phd Student: Khalili, Khadijeh (Intern)
Supervisor: Santra, Robin (Ekstern)
Main Supervisor: Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Implementation in real SOFC Systems of monitoring and diagnostic tools using signal analysis to increase their lifetime

Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 02/01/2017 → 31/12/2019
Number of participants: 1
Acronym: INSIGHT  
Project ID: INSIGHT  
Number of related Ph.D. students: 1  
Project participant:  
Hagen, Anke (Intern)  
Project  

**Commercial project SOFC related**  
Department of Energy Conversion and Storage  
Applied Electrochemistry  
Period: 02/01/2017 → 31/03/2017  
Number of participants: 1  
Project participant:  
Hagen, Anke (Intern)  
Project

**Nanofiber structures for efficient enzyme immobilization in membrane applications**  
International Network Project between DTU and Mahatma Gandhi University (MGU) and other partners from India  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Period: 01/01/2017 → 31/12/2017  
Number of participants: 1  
Membranes, electrospinning, water filtration, ceramic processing, nanofibers, enzymes  
Project ID: 6144-00035A  
Project participant:  
Kaiser, Andreas (Intern)  
Project

**The fabrication and testing of two terminal memristor device - Nano Ionic Conducting Engineered materials for information application**  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Electrofunctional materials  
Fundamental Electrochemistry  
ETH Zurich  
Period: 01/01/2017 → 31/01/2020  
Number of participants: 3  
Acronym: NICE  
Number of related Ph.D. students: 1  
Project participant:  
Esposito, Vincenzo (Intern)  
Traulsen, Marie Lund (Intern)  
Project Manager, organisational:  
Pryds, Nini (Intern)  
Project

**A novel off-grid thermoelectric-photovoltaic desalination system**  
Desalination of brackish water/sea water is a sustainable way to meet water demand in arid locations. A number of humidification/dehumidification (HDH) devices based on conventional vapor compression technology are currently available. However, these devices have a number of inherent problems such as high noise levels, compressor vibration and excessive weight and size.  
The overall objective of the project is to develop and demonstrate a novel off-grid desalination system using thermoelectric technology combined with a photovoltaic system.  
The combination of photovoltaic (PV) and thermoelectric (TE) technologies will not only overcome the problems of a
conventional desalination system, but it also brings many additional advantages such as being off-grid, having less moving parts, easy to install, less maintenance, and on top being environmentally friendly.

The outcome of the project will be:
(i) High performance thermoelectric-solar desalination prototype to cheaply produce potable water with a targeted coefficient of performance (COP) of more than 1.5.
(ii) Demonstration of a future environmentally friendly energy technological concept with high commercial potential.

In this project, DTU Energy, AquaDania A/S, SunPower Applications A/S, and All Things Considered A/S work closely together toward a goal to develop a novel off-grid desalination system using a thermoelectric module coupled with a PV system. We address the needs of people's drinking water in remote areas of the world, or the emergency needs of catastrophic situation especially people living in arid countries.

Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/01/2017 → 31/12/2018
Number of participants: 1
Acronym: NOVELTEC
Project Coordinator:
Van Nong, Ngo (Intern)

Solid Oxide Electrolysis Cell stack II
Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/01/2017 → 31/12/2017
Number of participants: 1
Acronym: SOEC II
Project participant:
Wulff, Anders Christian (Intern)

Advanced tailoring of 3D microstructures for superconducting magnets
Superconducting magnets capable of producing large magnetic fields are indispensable for magnetic resonance imaging (MRI) for medical diagnostics. The higher the field is, the higher the spatial resolution achievable in the scanner is; this is crucial for the early detection of, e.g., cancer tumors. The present research project focuses on a new concept for the superconducting magnet which will enable an increase in the magnetic field by a factor of more than three. This is done by using ceramic superconductors in combination with a novel substrate configuration recently developed by the applicant. The substrate makes it possible to produce many thin superconducting 3D structured filaments instead of a single wide conductor, thus increasing the field produced and improving the resolution of the MRI device. The project aims to solve the scientific problems currently impeding the achievement of sufficiently small filaments. A major scientific problem is related to oxygen formation and spread during electro-etching of 3D profiles resulting in undesired structural filament variations.

Department of Energy Conversion and Storage

Electrofunctional materials
Imaging and Structural Analysis
Period: 01/01/2017 → 01/01/2019
Number of participants: 7
surface modification, electrochemistry, topography, Coated conductor, Superconductor, ceramic processing
Acronym: ATOMIS
Project ID: DFF – 6111-00252)
Project participant:
Insinga, Andrea Roberto (Intern)
Grivel, Jean-Claude (Intern)
Nielsen, Pernille Hedemark (Intern)
Wichmann, Mike (Intern)
Usoskin, Alexander (Ekstern)
Gömöry, Fedor (Ekstern)
Project Manager, academic:
Wulff, Anders Christian (Intern)
Project
Adhesive development for flexible thin film electronic encapsulation

Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Kovrov, Aleksandr (Intern)
Supervisor:
Helgesen, Martin (Intern)
Main Supervisor:
Sendergaard, Roar R. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Density functional theory based modelling of materials for resistive switching memories

Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 4
Phd Student:
Pedersen, Christian Sendergaard (Intern)
Supervisor:
Pryds, Nini (Intern)
Vegge, Tejs (Intern)
Main Supervisor:
García Lastra, Juan Maria (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

DronEL

The purpose of this project is to develop and bring to market an aerial drone based automated solution (DronEL) used for a full PV plant survey for more accurate survey in less time. The automatic drone-based inspection method combines IR, EL and PL imaging, and visual images.

Department of Photonics Engineering
Diode Lasers and LED Systems
Coding and Visual Communication
Centre of Excellence for Silicon Photonics for Optical Communications
Department of Energy Conversion and Storage
Organic Energy Materials
Aalborg University
Sky Watch
SiCon
Kenergy
Skive Kommune
Period: 01/01/2017 → 31/12/2019
Number of participants: 8
Project ID: 71001
Project participant:
Thorsteinsson, Sune (Intern)
Forchhammer, Søren (Intern)
Benatto, Gisele Alves dos Reis (Intern)
Riedel, Nicholas (Intern)
Thorseth, Anders (Intern)
Dam-Hansen, Carsten (Intern)
Mantel, Claire (Intern)
Project Manager, organisational:
Poulsen, Peter Behrensdorff (Intern)

Relations
Related projects:

PV LED ENGINE
PV BALCONY FENCE – a highly esthetic cost efficient PV integrated balcony
Activities:
7th International SpectroRadiometer Comparison (ISRC 2017)
Activities in the standardisation of light sources and spectroradiometer calibration
Publications:
New dental applications with LEDs
Quantification of solar cell failure signatures based on statistical analysis of electroluminescence images
Luminescence Imaging Strategies for Drone-Based PV Array Inspection
Indoor measurement of angle resolved light absorption by antireflective glass in solar panels
New Light Source Setup for Angle Resolved Light Absorption measurement of PV sample
Optimizing sensitivity of Unmanned Aerial System optical sensors for low zenith angles and cloudy conditions
Development of outdoor luminescence imaging for drone-based PV array inspection

Project

Freeze casting to create micro-channel structures
Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Christiansen, Cathrine Deichmann (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Main Supervisor:
Bjørk, Rasmus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Theoretical investigations of the sudden death process in metal-air batteries
Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Tygesen, Alexander Sougaard (Intern)
Supervisor:
Vegge, Tejs (Intern)
Main Supervisor:
Garcia Lastra, Juan Maria (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Advanced neutron imaging of energy devices in 2D and 3D

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 4
Phd Student: Lacatusu, Monica-Elisabeta (Intern)
Supervisor: Schmidt, Søren (Intern)
Strobl, Markus (Ekstern)
Main Supervisor: Kuhn, Luise Theil (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Improving the interface adherence in solid oxide fuel cell stacks

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 4
Phd Student: Ritucci, Ilaria (Intern)
Supervisor: Agersted, Karsten (Ekstern)
Frandsen, Henrik Lund (Intern)
Main Supervisor: Kiebach, Wolff-Ragnar (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Solid oxide fuel cells and biogas

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 3
Phd Student: Langnickel, Hendrik (Intern)
Supervisor: Olsen, Rasmus (Ekstern)
Main Supervisor: Hagen, Anke (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Novel Anodes for Solid Oxide Fuel Cells

Department of Energy Conversion and Storage
Period: 01/11/2016 → 31/10/2019
Number of participants: 4
Phd Student:
Novel Cobalt Free Oxygen Electrodes for Solid Oxide Electrolysis Cells

Department of Energy Conversion and Storage
Period: 01/11/2016 → 31/10/2019
Number of participants: 4
Phd Student: Tong, Xiaofeng (Intern)
Supervisor: Hendriksen, Peter Vang (Intern)
Main Supervisor: Ovtar, Simona (Intern)
Chen, Ming (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institutt stipendie (DTU)
Project: PhD

Cost and energy effective all-black solar cell panel | Black Si BIPV | Phase 2

The objective of the EUDP project is to develop and manufacture a novel type of solar panel based on a new type of solar cell (black silicon solar cell), which – apart from a high and preferably improved efficiency and an implementable and cheaper production method – should have several significant advantages in terms of building integration. The black solar cells will be further processed to make the front conducting grid completely black through an electrochemical deposition technology. The tabbing wires interconnecting the cells in the panel will be processed into non-reflecting black strings in a scalable, inorganic electrochemical process step securing a completely black appearance of the solar panel later produced. A compatible panel production process with traditional PV panel process will be demonstrated for the total black silicon BIPV module.

Department of Photonics Engineering
Diode Lasers and LED Systems
Department of Micro- and Nanotechnology
Silicon Microtechnology
Experimental Surface and Nanomaterials Physics
Department of Energy Conversion and Storage
Organic Energy Materials
Gaia Solar A/S
Institute for Product Development
SoliTek
Nines Photovoltaics
Period: 01/10/2016 → 30/09/2018
Number of participants: 7
BIPV, Black Silicon
Acronym: BS2
Project participant: Thorsteinsson, Sune (Intern)
Highly defective oxides – the next generation of electromechanical materials

Materials capable of changing shape in response to an electrical field work as muscles and have important applications as actuators in many different contexts. At present, the most widely used materials contain lead (Pb) which is highly toxic. Recently, an entirely new class of electromechanically active materials has been discovered: highly defective cerium oxides, i.e. ceria with a large concentration of oxygen vacancies in the crystal lattice. Such materials contain no toxic elements and have a giant electromechanical response even under moderate electric fields. Governed by a still unexplored atomistic mechanism, the main underlying phenomenon seems to be the organization of the oxygen vacancies. This effect is observed so far only in thin films (below 1 micron) in textured microstructures, but in order to replace the current lead-based actuator materials the properties have to be brought to the level of thick films and bulk components. To this scope, the GIANT-E project has 2 success criteria, namely: (1) Understanding the fundamental effect of the film thickness on the electrostrictive properties of highly defective oxides; (2) Identifying a methodology for stabilizing the electromechanical properties in bulk by tailoring microstructure and oxygen defects. Such results will lay the foundations for a new paradigm of bulk lead-free electromechanically active materials for multi-scale applications. The concept will be tested by a Danish industrial player, NOLIAC, for biomedical applications.

Department of Energy Conversion and Storage

Ceramic Engineering & Science

Weizmann Institute of Science

Period: 01/09/2016 → 31/08/2019

Number of participants: 1

Acronym: GIANT-E

Project participant:

Esposito, Vincenzo (Intern)

Project
Hauch, Anne (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Chen, Ming (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Nano-Editor: Development of nano-materials based printing media for all-ceramic solid oxide fuel cells manufacturing

Department of Energy Conversion and Storage
Period: 01/09/2016 → 31/08/2019
Number of participants: 3
Phd Student:
Rosa, Massimo (Intern)
Supervisor:
Zielke, Philipp (Intern)
Main Supervisor:
Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

X-ray phase contrast nano-tomography of 3rd generation solar cells

Department of Energy Conversion and Storage
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Fevola, Giovanni (Intern)
Supervisor:
Carbone, Gerardina (Ekstern)
Dong, Yiqiu (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Electrodeposition of Metallic 3D Surface-Profiles for Superconductor Tapes

Master thesis project by Suzanne Zamany Andersen. Thesis abstract: The work in this thesis is based on a recently introduced 3D surface-prole technique, i.e. the two-level undercut-prole substrate (2LUPS) concept [1]-[2], used for production of multi-lamentary high-temperature coated conductor (CC) tapes. Reducing the superconductor lament width linearly reduces the alternating current hysteretic energy losses [3], and it enables manufacturing of stable high-temperature superconducting magnets [4]. A new process of tape masking and Ni-based electroplating on a Ni-W metal alloy substrate to form similar 3D surfacepro les as those achieved by the 2LUPS concept [5], which is based on two levels of plateaus connected via an undercut-prole, is investigated. The undercut-prole should be large enough to enable a shading eect during subsequent physical vapor deposition (PVD) of layers, thereby creating self-formed and physically separated superconductor laments on the two plateaus, while still utilizing the full width of the CC. This will theoretically increase the engineering current density compared to current lament techniques utilizing e.g. laser striation or mechanical scribing. Inspection of the metal substrate cross-section using focused ion beam milling and scanning electron microscopy (FIBSEM) reveals that an undercut-prole is achieved by using kapton tape as a mask while electroplating nickel to create the upper plateaus. The arithmetic surface roughness of the electroplated nickel layer is determined via atomic force microscopy (AFM) to be suitable for CC fabrication. To verify if the undercut-prole is sucient, an electrically insulating layer of SiO, simulating the buer layers in CCs, followed by an electrically conductive layer of Ag, simulating the superconducting layer, is deposited using PVD, and four-point probe measurements to create I/V characteristics are used to measure resistance across plateaus. The plateaus are deemed electrically insulated from each other, as the
resistances from each insulating layer adds up to the total resistance through both plateaus. Accordingly, it is expected that these new electroplated 3D surface-profiles will also enable lamentization of superconductors produced by PVD processes. A small caveat to these findings, is the lack of a suitable profile for the use in CC fabrication being manufactured in this project. The adhesive in the masking tape creates bulges or protrusions in the profile, so a further study on thinner adhesive layers or a different masking material altogether is needed. The possibility of texture transfer from the Ni-W metal substrates to the plated Ni layer is also investigated, for the use in the cheaper rolling assisted bi-axially textured substrate (RABiTS) fabrication process. The electrodeposited Ni would during annealing at low temperatures experience an abnormal grain growth stage, thereby rendering it incapable of attaining the texture needed for RABiTS fabrication. Furthermore, the thermal grooving during annealing of the pure Ni could also become a problem for the ion beam assisted deposition (IBAD) process, as a surface roughness of <5nm is desired. The author of this thesis therefore strongly recommends investigating the possibility of plating e.g. Ni-W instead.

Department of Energy Conversion and Storage

Electrofunctional materials

Department of Physics

Experimental Surface and Nanomaterials Physics

Imaging and Structural Analysis
Period: 22/08/2016 → 12/02/2017
Number of participants: 5
electrochemistry, electroplating, metal substrates, Coated conductor, Superconductor, topography, EBSD, FIB-SEM, texture
Project participant:
Andersen, Suzanne Zamany (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Nielsen, Pernille Hedemark (Intern)
Main Supervisor:
Wulff, Anders Christian (Intern)
Examiner:
Bentien, Anders (Ekstern)
Project

Advanced structuring of adsorbents by electrospinning for gas cleaning and storage

Department of Energy Conversion and Storage
Period: 15/08/2016 → 15/08/2017
Number of participants: 4
Phd Student:
Vinkel, Nadja Maria (Intern)
Supervisor:
Akhtar, Farid (Ekstern)
Zhang, Wenjing (Angela) (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Co-electrolysis SOEC

Department of Energy Conversion and Storage
Period: 15/08/2016 → 14/08/2019
Number of participants: 3
Phd Student:
Rao, Megha (Intern)
Supervisor:
Sun, Xiuju (Intern)
Main Supervisor:
Hagen, Anke (Intern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: **Anden EU-finansiering**  
Project: PhD

**Computational design of catalysts for electroreduction of nitrogen into ammonia**

Department of Energy Conversion and Storage  
Period: 01/08/2016 → 31/07/2019  
Number of participants: 3  
Phd Student:  
Pan, Jaysree (Intern)  
Supervisor:  
Hansen, Heine Anton (Intern)  
Main Supervisor:  
Vegge, Tejs (Intern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: **Eksternt finansieret virksomhed**  
Project: PhD

**Density Functional Theory Studies of Water Electrolysis on Ceria**

Department of Energy Conversion and Storage  
Period: 01/08/2016 → 31/07/2019  
Number of participants: 3  
Phd Student:  
Wu, Tiantian (Intern)  
Supervisor:  
Hansen, Heine Anton (Intern)  
Main Supervisor:  
Vegge, Tejs (Intern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: **Eksternt finansieret virksomhed**  
Project: PhD

**Cost-effective and flexible 3D printed SOFC stacks for commercial applications**

A Solid Oxide Fuel Cell (SOFC) is a ceramic-based multilayer device that involves expensive and time-consuming multi-step manufacturing processes including tape casting, screen printing, firing, shaping and several high-temperature thermal treatments. In addition, these cells are manually assembled into stacks resulting in extra steps for joining and sealing that difficult the standardization and quality control of the final product while introducing weak parts likely to fail. Since current ceramics processing presents strong limitations in shape and extremely complex design for manufacturing (more than 100 steps), industrially fabricated SOFC cells and stacks are expensive and present low flexibility and long time to market. This is particularly relevant for the commercial segment of the stationary fuel cells market (5-400kW) that is highly heterogeneous in terms of the overall power and heat requirements and requires customization of the final product. The main goal of the Cell3Ditor project is to develop a 3D printing technology for the industrial production of SOFC stacks by covering research and innovation in all the stages of the industrial value chain (inks formulation, 3D printer development, ceramics consolidation and system integration). All-ceramic joint-free SOFC stacks with embedded fluidics and current collection will be fabricated in a two-step process (single-step printing and sintering) to reduce in energy, materials and assembly costs while simplifying the design for manufacturing and time to market. Compared to traditional ceramic processing, the Cell3Ditor manufacturing process presents a significantly shorter time to market (from years to months) and a cost reduction estimated in 63% with an initial investment below one third of an equivalent conventional manufacturing plant (production of 1000 units per year). The project is product-driven and involves SMEs (with proved technologies) in the entire value chain to ensure reaching TRL>6.

Department of Energy Conversion and Storage  
Ceramic Engineering & Science
Breaking the temperature limits of Solid Oxide Fuel Cells: Towards a new family of ultra-thin portable power sources

Solid Oxide Fuel Cells (SOFCs) are one of the most efficient and fuel flexible power generators. However, a great limitation on their applicability arises from temperature restrictions. Operation approaching room temperature (RT) is forbidden by the limited performance of known electrolytes and cathodes while typical high temperatures (HT) avoid their implementation in portable applications where quick start ups with low energy consumption are required.

The ULTRASOFC project aims breaking these historical limits by taking advantage of the tremendous opportunities arising from novel fields in the domain of the nanoscale (nanoionics or nano photochemistry) and recent advances in the marriage between micro and nanotechnologies. From the required interdisciplinary approach, the ULTRASOFC project addresses materials challenges to (i) reduce the operation to RT and (ii) technological gaps to develop ultra-low-thermal mass structures able to reach high T with extremely low consumption and immediate start up.

A unique µSOFC technology fully integrated in ultrathin silicon will be developed to allow operation with hydrogen at room temperature and based on hydrocarbons at high temperature. Stacking these µSOFCs will bring a new family of ultrathin...
power sources able to provide 100 mW at RT and 5W at high T in a size of a one-cent coin. A stand-alone device fuelled with methane at HT will be fabricated in the size of a dice. Apart from breaking the state-of-the-art of power portable generation, the ULTRASOFC project will cover the gap of knowledge existing for the migration of high T electrochemical devices to room temperature and MEMS to high T. Therefore, one should expect that ULTRASOFC will open up new horizons and opportunities for research in adjacent fields like electrochemical transducers or chemical sensors. Furthermore, new technological perspectives of integration of unconventional materials will allow exploring unknown devices and practical applications.

Department of Energy Conversion and Storage

Ceramic Engineering & Science
Period: 01/04/2016 → 31/03/2021
Number of participants: 2
Acronym: ULTRA-SOFC.
Project participant:
Esposito, Vincenzo (Intern)
Project Manager, organisational:
Taracón, Albert (Ekstern)

Active Magnetic regenerator refrigeration with rotary multi-bed technology

Department of Energy Conversion and Storage
Period: 01/04/2016 → 20/09/2016
Number of participants: 7
Phd Student:
Eriksen, Dan (Intern)
Supervisor:
Bahl, Christian (Intern)
Bjørk, Rasmus (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Jensen, Jens Oluf (Intern)
Kitanovski, Andrej (Ekstern)
Palm, Björn (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Active magnetic regenerator refrigeration with rotary multi-bed technology
Project: PhD

Commercial project SOFC related

Department of Energy Conversion and Storage

Applied Electrochemistry
Period: 01/04/2016 → 31/03/2017
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Highly structured materials for upgraded biogas and storage
HiGradeGas will develop nanostructured materials for more efficient adsorption processes to remove CO₂ from biogas (upgrading) and to store the resulting biomethane.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
SINTEF
Stockholm University
Syddansk Universitet
Danish Power Systems ApS
NeoZeo AB
Rambøll Oil and Gas
Lulea University of Technology
Period: 01/03/2016 → 29/02/2020
Number of participants: 1
Biogas upgrading, pressure swing adsorption, Nanofibers, gas adsorption
Acronym: HiGradeGas
Number of related Ph.D. students: 2
Project Coordinator:
Kaiser, Andreas (Intern)

3D Imaging center
Department of Physics
Neutrons and X-rays for Materials Physics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Electrofunctional materials

Centre for oil and gas – DTU
Period: 01/01/2016 → 01/01/2021
Number of participants: 14
Project participant:
Dahl, Anders Bjørholm (Intern)
Oddershede, Jette (Intern)
Trinderup, Camilla Himmelstrup (Intern)
Simonsen, Søren Bredmose (Intern)
Zheng, Yi (Intern)
Brink, Bastian (Intern)
Lauridsen, Torsten (Ekstern)
Thydén, Karl Tor Sune (Intern)
Sanna, Simone (Intern)
Baier, Sina (Intern)
Bentzen, Janet Jonna (Intern)
Christensen, Anders Nymark (Intern)
Project Manager, organisational:
Gundlach, Carsten (Intern)
Project Manager, academic:
Poulsen, Henning Friis (Intern)

Related projects:
Alliance for Imaging and Modelling of Energy Applications
Publications:
From concept to in vivo testing: Microcontainers for oral drug delivery
Scene reassembly after multimodal digitization and pipeline evaluation using photorealistic rendering
Graphite nODULES in fatigue-tested cast iron characterized in 2D and 3D
In-Situ X-ray Tomography Study of Cement Exposed to CO₂ Saturated Brine
Crack Tip Flipping under Mode I Tearing: Investigated by X-Ray Tomography
Powder embossing method for selective loading of polymeric microcontainers with drug formulation
High-Performance Microchanneled Asymmetric Gd₀.₁Ce₀.₉O₁.ₙ₅-₅-La₀.₆Sr₀.₄FeO₃-₅-Based Membranes for Oxygen Separation
Characterization of graphite NODULES in thick-walled ductile cast ir-ons
Surface Detection using Round Cut
Microstructure and micromechanics of the heart urchin test from X-ray tomography
Synthesis and characterization of Fe–Ni/γ-Al₂O₃ egg-shell catalyst for H₂ generation by ammonia decomposition

High Temperature Superconducting Bolometer

Department of Energy Conversion and Storage
Electrofunctional materials
Department of Physics
Quantum Physics and Information Technology
Department of Photonics Engineering
Period: 01/01/2016 → 31/08/2016
Number of participants: 3
Superconductor
Supervisor:
Jepsen, Peter Uhd (Intern)
Main Supervisor:
Wulff, Anders Christian (Intern)

SOFC stack project

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2016 → 31/12/2016
Number of participants: 1
Project participant:
Wulff, Anders Christian (Intern)

New Thermoelectric Materials

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2016 → …
Number of participants: 1
Acronym: NeTeMa
Project Coordinator:
Van Nong, Ngo (Intern)

Thermal Energy Storage - Lab-Scale prototype
Large quantities of thermal energy – both per weight and price - can be stored reversibly in many salts upon ab-/desorption of water or ammonia. The project is to develop thermochemical heat storage (TCS) system based on NH₃ ab/desorption in metal halides. We target for this lab-scale prototype a storage capacity of 1 MJ (2.5 kg NH₃) based first on existing mixed metal salts (e.g. SrBaCl₂), to demonstrate the system feasibility and document the actual efficiency of the different components and test the mechanical and structural properties of the system during multiple cycles.
Department of Energy Conversion and Storage

Atomic scale modelling and materials
Period: 01/01/2016 → 01/01/2018
Number of participants: 1
Thermal Energy Storage, Thermo chemical energy storage, ammonia
Acronym: TES
Project participant:
Blanchard, Didier (Intern)

High Efficiency Thermoelectric Module
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2016 → ...
Number of participants: 1
Acronym: HiTEM
Project Coordinator:
Van Nong, Ngo (Intern)

Development of a new synthesis for highly active fuel cell electrocatalysis
Department of Energy Conversion and Storage
Period: 15/12/2015 → 14/12/2018
Number of participants: 4
Phd Student:
Brandes, Benedikt Axel (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Improving the efficiency of heat pump and cooling technologies
Department of Energy Conversion and Storage
Period: 15/12/2015 → 14/12/2018
Number of participants: 3
Phd Student:
Navickaitė, Kristina (Intern)
Supervisor:
Bahl, Christian (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Development and characterization of emerging battery electrodes and electrolytes
Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Lefevr, Jessica (Intern)
Supervisor:
Hoster, Harry Ernst (Ekstern)
Norby, Poul (Intern)
Main Supervisor:
Blanchard, Didier (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Activities:
Hydrides as Energy Materials
10th International Symposium "Hydrogen & Energy"
Lithium-Sulfur Solid-State Batteries Based on Nanoconfined LiBH4
Project: PhD

Electrical Properties of Correlated Electron Systems at the Interfaces of Complex Oxides
Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
von Soosten, Merlin (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Jespersen, Thomas Sand (Ekstern)
Main Supervisor:
Pryds, Nini (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Improvement of Electrode Materials for High temperature Electrolysis Cells
Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Tripkovic, Dordije (Intern)
Supervisor:
Bilge, Yildiz (Ekstern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Hendriksen, Peter Vang (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Next generation rechargeable batteries: Sustainable and earth-abundant materials
Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018  
Number of participants: 4  
Phd Student: 
Christensen, Mathias Kjærgård (Intern)  
Supervisor: 
Hoster, Harry Ernst (Ekstern)  
Vege, Tejs (Intern)  
Main Supervisor: 
Norby, Poul (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

**Improvement of Cell Strength in High Temperature Electrolysis Cells**  
Department of Energy Conversion and Storage  
Period: 01/11/2015 → 31/10/2018  
Number of participants: 3  
Phd Student: 
Khajavi, Peyman (Intern)  
Supervisor: 
Hendriksen, Peter Vang (Intern)  
Main Supervisor: 
Frandsen, Henrik Lund (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis**  
Department of Energy Conversion and Storage  
Period: 15/10/2015 → 14/10/2018  
Number of participants: 4  
Phd Student: 
Fenini, Filippo (Intern)  
Supervisor: 
Kammer Hansen, Kent (Intern)  
Hendriksen, Peter Vang (Intern)  
Main Supervisor: 
Mogensen, Mogens Bjerg (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Development of non-precious metal polymer fuel cell catalysts**  
Department of Energy Conversion and Storage  
Period: 15/09/2015 → 14/09/2018  
Number of participants: 4  
Phd Student: 
Shypunov, Illia (Intern)  
Supervisor: 
Cleemann, Lars Nilausen (Intern)  
Li, Qingfeng (Intern)  
Main Supervisor:
**Modeling Energy Supply for Future Cities**

Department of Energy Conversion and Storage  
Period: 15/09/2015 → 14/09/2018  
Number of participants: 4  
Phd Student:  
Dominkovic, Dominik Franjo (Intern)  
Supervisor:  
Nielsen, Per Sieverts (Intern)  
Sørensen, Mads Peter (Intern)  
Main Supervisor:  
Pedersen, Allan Schrøder (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Relations**  
Activities:  
Blockchain Summer School 2017  
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017  
12th International SDEWES Conference  
The 40th International IAEE Conference  
30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems

**Publications:**  
Potential for dynamic pricing in district heating systems in Denmark and Finland  
Integration of district cooling in smart energy systems: the case of Singapore

**Nano-scale 3D reconstruction of phase contrast X-ray projections**

Department of Energy Conversion and Storage  
Period: 15/09/2015 → 14/09/2018  
Number of participants: 3  
Phd Student:  
Cunha Ramos, Tiago Joao (Intern)  
Supervisor:  
Jørgensen, Jakob Sauer (Intern)  
Main Supervisor:  
Andreasen, Jens Wenzel (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)  
Project: PhD

**ESS & MAX IV: Cross border science and society**  
Workpackage: ESS & MAX IV: Cross border network and post graduate educational program  
Department of Energy Conversion and Storage  
Imaging and Structural Analysis  
Department of Physics
SOFC degradation studies
Department of Energy Conversion and Storage
Period: 15/08/2015 → 14/08/2018
Number of participants: 3
PhD Student:
Ploner, Alexandra (Intern)
Supervisor:
Hauch, Anne (Intern)
Main Supervisor:
Hagen, Anke (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Development and characterization of novel high temperature and pressure alkaline electrolysis cells (HTP-AEC)
Department of Energy Conversion and Storage
Period: 01/08/2015 → 31/08/2018
Number of participants: 4
PhD Student:
Adolphsen, Jens Quitzau (Intern)
Supervisor:
Gil, Vanesa (Intern)
Sudireddy, Bhaskar Reddy (Intern)
Main Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Multilayer inorganic structures for high performance enzyme immobilization and separation
Department of Energy Conversion and Storage
Period: 01/08/2015 → 30/11/2015
Number of participants: 4
Phd Student:
Ghannadi, Saber (Intern)
Supervisor:
Kaiser, Andreas (Intern)
Pinelo, Manuel (Intern)
Main Supervisor:
Della Negra, Michela (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Dark Field X-ray Microscopy of energy materials
Department of Energy Conversion and Storage
Period: 15/06/2015 → 14/07/2018
Number of participants: 4
Phd Student:
Sierra Trujillo, José Xavier (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Poulsen, Henning Friis (Intern)
Main Supervisor:
Bowen, Jacob R. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis cells
Department of Energy Conversion and Storage
Period: 15/06/2015 → 31/07/2015
Number of participants: 4
Phd Student:
Hausladen, Mathias (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Ramos, Tania (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Electrochemical Characterization for Improvement of PEM Electrolyzers for Flexible Energy Storage
Department of Energy Conversion and Storage
Period: 15/06/2015 → 14/06/2018
Number of participants: 4
Phd Student:
Elsøe, Katrine (Intern)
Supervisor:
Hjelm, Johan (Intern)
Ramos, Tania (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

High Current All Printed Transistors
The fast evolution of printed electronics, with the photovoltaic technology in primis, is requiring the presence of a valid transistor alternative to the traditional one. The realization of a high current roll-to-roll transistor will interconnect all the different technologies so far developed with this low cost and high throughput method. Our aim is to develop a roll-to-roll transistor capable to of modulate the current to levels that has not been achieved so far. The fabrication of the transistor will be done considering the lowest environmental impact possible, and containing energy consumption with a temperature below 150 °C. This high current (~mA) transistor will be able to support and assist other technologies and will also be the base for logics and sensing application. The optical studies on the organic material will result in a more controllable production process that for the first time will relate polymer crystallinity directly with an optical characterization technique. The realization of such kind of measurements is not trivial, but will give information on polymer nanoscale structures never investigated before. To do so this technique uses femtosecond pulse in subdiffraction-limited area. This will disclose an unprecedented tool to control the polymer morphology as soon as it is deposited, with enormous consequences in performance control and optimization. The realization of samples and the study of real cases will produce important information regarding this new technology and its real life applications. In addition, life-time and stability studies can be performed. Then the objective of minimizing the environmental impact of the technology life time cycle will be more realistic. These kinds of studies are also important to explain science to the society and to give a technology preview to industries.

Department of Energy Conversion and Storage
Organic Energy Materials
Period: 01/05/2015 → …
Number of participants: 1
printed, electronics, smart, windows, Solar Cells, Organic
Acronym: HCAPT
Project ID: 659747
Project participant:
Pastorelli, Francesco (Intern)
Documents:
European Commission _ CORDIS _ Projects and Results _ High Current All Printed Transistors

New composite materials for high temperature water splitting and synthetic fuel production by solar thermochemical conversion
In this project we propose a novel concept material for high temperature H2O/CO2 splitting based on a porous ceramic composite comprised of high-temperature ceramics and cerium oxide in its highly doped form. In the composite, the low diffusivity at the refractory component inhibits the mass diffusion mechanisms in the catalytic component (doped-ceria), thus preserving the microstructure from the detrimental densification effects.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/05/2015 → 31/03/2018
Number of participants: 1
Acronym: HT-COMPO
Project Coordinator:
Esposito, Vincenzo (Intern)

In-operando spatially resolved probing of solid oxide electrolysis/fuel cells

Department of Energy Conversion and Storage
Period: 01/05/2015 → 30/04/2018
Number of participants: 5
Phd Student:
Pitscheider, Simon (Intern)
Supervisor:
Chueh, William C. (Ekstern)
Hansen, Karin Vels (Intern)
Hjelm, Johan (Intern)
Main Supervisor:
Chatzichristodoulou, Christodoulos (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Young investigator Program from Villum Foundation
Department of Energy Conversion and Storage
Period: 01/05/2015 → 10/09/2018
Number of participants: 4
Phd Student:
Mathiesen, Nicolai Rask (Intern)
Supervisor:
Vegge, Tejs (Intern)
Vegge, Tejs (Intern)
Main Supervisor:
García Lastra, Juan Maria (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

SOFC Testing Part 1 and 2
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 13/04/2015 → 31/10/2015
Number of participants: 2
Project participant:
Hagen, Anke (Intern)
Sun, Xiufu (Intern)

Density Functional Theory Studies of the Oxygen Reduction Reaction on Non-Precious Electrodes
Department of Energy Conversion and Storage
Period: 01/04/2015 → 31/03/2018
Number of participants: 3
Phd Student:
Reda, Mateusz (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
In-operando localized probing of solid oxide electrolysis/fuel cells by controlled atmosphere high temperature scanning probe microscopy

Department of Energy Conversion and Storage
Period: 15/03/2015 → 14/03/2018
Number of participants: 5
Phd Student:
Kreka, Kosova (Intern)
Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Mogensen, Mogens Bjerg (Intern)
Norman, Kion (Intern)
Main Supervisor:
Hansen, Karin Vels (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

The role of contact resistance in thermoelectric module

Department of Energy Conversion and Storage
Period: 15/02/2015 → 01/08/2018
Number of participants: 5
Phd Student:
Malik, Safdar Abbas (Intern)
Supervisor:
Stamate, Eugen (Intern)
Nielsen, Kaspar Kirstein (Intern)
Pryds, Nini (Intern)
Main Supervisor:
Van Nong, Ngo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Demonstration af Danmarks Fremtidige Energisystem i Miniformat

Department of Energy Conversion and Storage

Applied Electrochemistry
Period: 19/01/2015 → 31/12/2015
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Filamentary Coated Conductors

Internal DTU Energy project about superconducting tapes; Main objective is to develop a strongly cube textured two-level-undercut-profile-substrate for filamentary coated conductors.

Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/01/2015 → 31/12/2015
Number of participants: 1
Project participant:
Wulff, Anders Christian (Intern)

Project

Rare-earth/transition-metal oxides and compounds for environment-friendly energy science and technology
This network programme is to setup win-win scientific collaborations between the DTU Energy Conversion and the State Key Laboratory of Magnetism (SKLM), Institute of Physics (IOP), Chinese Academy of Sciences (CAS) in Beijing, China. This is expected to improve largely the core competences for both the Danish and the Chinese partners, known for advanced energy conversion technology and excellent fundamental research, respectively.

Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/01/2015 → 31/12/2015
Number of participants: 1

Magnetic Cooling, Oxide Interfaces
Project participant:
Chen, Yunzhong (Intern)

Acid-base chemistry and HT-polymer electrolyte membranes
Department of Energy Conversion and Storage
Period: 15/12/2014 → 14/12/2017
Number of participants: 3
Phd Student:
Becker, Hans (Intern)
Supervisor:
Jensen, Jens Oluf (Intern)
Main Supervisor:
Li, Qingfeng (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Advanced nano-inks for ink-jet printing of functional metal oxides for energy and environment devices - Smart Inks
Department of Energy Conversion and Storage
Period: 15/12/2014 → 14/12/2017
Number of participants: 6
Phd Student:
Gadea, Christophe (Intern)
Supervisor:
Ramousse, Severine (Intern)
Main Supervisor:
Esposito, Vincenzo (Intern)
Examiner:
Tavacoli, Joe (Intern)
De Buysser, Klaartje (Ekstern)
Sanson, Alessandra (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

ECOdesign of urban buildings by integration of organic photovoltaics microgrids (ECLIPS microgrids)
Department of Energy Conversion and Storage
Period: 15/12/2014 → 14/12/2017
Number of participants: 4
Analysis of Fracture in Porous Ceramic Catalysts by use of X-ray Tomography

Department of Energy Conversion and Storage
Period: 01/12/2014 → 13/05/2018
Number of participants: 5
Phd Student:
Jacobson, Hjalte Sylvest (Intern)
Supervisor:
Molina, Anna M. Puig (Ekstern)
Poulsen, Henning Friis (Ekstern)
Sørensen, Bent F. (Intern)
Main Supervisor:
Frandsen, Henrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of High temperature PEM fuel cells

Department of Energy Conversion and Storage
Period: 15/11/2014 → 14/11/2017
Number of participants: 5
Phd Student:
Kannan, Arvind (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)
Examiner:
Bjerrum, Niels J. (Intern)
Andreasen, Søren Juhl (Ekstern)
Zeis, Roswitha (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Topology optimization of thermal heat sinks
PhD Project
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Mechanical Engineering
Solid Mechanics
In situ transmission electron microscopy on operating electrochemical cells

Solid oxide fuel/electrolysis cells (SOFC/SOEC) will play an important role in future efficient and environmentally friendly energy systems if a better long term performance of the cells can be achieved. In a solid oxide fuel cell (SOFC) a fuel such as hydrogen, methane, synthesis gas, etc. is oxidized over a solid oxygen ion-conducting electrolyte which physically separates fuel and air.

The electron transfer in this chemical reaction takes place via an external circuit and electricity is therefore a product of the reaction. Catalysts are used on both sides of the ion conducting electrolyte to activate the splitting of fuel and oxygen molecules.

Impressive performance improvements have recently been reported for cells with specific multiphase nano-structures, but structural and compositional nano-scaled changes can also lead to deactivation. On the other hand, deactivation processes due to nano-scaled structural and compositional changes (segregations followed by nano-particle precipitation in some cases) can be observed near the material interfaces in the electrodes. Neither the mechanisms of the initial fast electrode process nor the development and dynamics of these critical structures are understood. Further studies of these dynamical changes are hampered since there are no available methods which offer in situ characterization of operating cells with nano-scale spatial resolution.

The project will develop a method for in situ transmission electron microscopy (TEM) of operating solid oxide electrochemical cells. Until now, knowledge of the nanoscale SOFC/SOEC dynamics is entirely based on observations performed post mortem, when the cells have been cooled down and de-mounted. To obtain direct insight into the dynamics of the active nanostructures of a SOFC/SOEC in operation can therefore have significant importance for our understanding of the cell dynamics during activation and deactivation.

The aim is to record TEM image sequences (movies) with atomic resolution of the active nanostructures in the SOFC/SOEC during operation. To do this, model SOFC/SOEC systems will be developed and integrated into a TEM
holder so that heating, electrical currents and exposure to reactive gas environments all are integrated at the same time. In addition the model systems will need to be highly compact and the thickness of the imaged area should be approximately 100 nm. The project will therefore push the limits of in situ TEM experiments.

The goal is direct insight into the nano-scale dynamics of the operating SOFC/SOEC during exposure to elevated temperatures, electrical currents and a reactive gas environment. This will be a key factor in developing more efficient and stable SOFCs/SOECs. Therefore, micro-SOFC will be developed and characterized by thin layer, especially regarding the electrolyte layer which will have a thickness lower than one micrometre. This will allow to work at temperature lower than 600°C.

The project will be carried out as a PhD project in collaboration between the two applicant institutions (DTU Energy Conversion and DTU Cen) and with the in situ group from Nagoya University with Prof. Shunsuke Muto. The work will primarily be carried out by the PhD student with support and supervision from the project team. The principal supervisor is Head of Section Luise T. Kuhn. The TEM work will be carried out under the guidance of Søren Bredmose Simonsen and Prof. Jakob B. Wagner. Prof. Mogens B. Mogensen will contribute to the project as an internal consultant when analyzing and linking the observed physical properties to the electrochemical performance.

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Center for Electron Nanoscopy
DTU Danchip
Period: 01/10/2014 → 30/09/2017
Number of participants: 4
In-situ TEM, fuel cell, electrolysis, electrochemistry, Nanotechnology
Acronym: TEMOC
Number of related Ph.D. students: 1
Project participant:
Kuhn, Luise Theil (Intern)
Simonsen, Søren Bredmose (Intern)
Wagner, Jakob Birkedal (Intern)
Gualandris, Fabrizio (Intern)

In-situ transmission electron microscopy on operating electrochemical cells
Department of Energy Conversion and Storage
Period: 01/10/2014 → 30/09/2017
Number of participants: 7
Phd Student:
Gualandris, Fabrizio (Intern)
Supervisor:
Simonsen, Søren Bredmose (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Kuhn, Luise Theil (Intern)
Examiner:
Bowen, Jacob R. (Intern)
Sharma, Renu (Ekstern)
Wallenberg, Reine (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Graded Oxygen Transport Membranes for Carbon Capture Processes
Department of Energy Conversion and Storage
Period: 15/09/2014 → 14/09/2017
Number of participants: 7
Phd Student:
Pirou, Stéven (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Kaiser, Andreas (Intern)
Main Supervisor:
Kiebach, Wolff-Ragnar (Intern)
Examiner:
AGERSTED, Karsten (Ekstern)
Baumann, Stefan (Ekstern)
Kriegel, Ralf (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering

**Relations**
Publications:

Development of Dual-Phase Oxygen Transport Membranes for Carbon Capture Processes
Project: PhD

**Studies of doping effects on the superconducting properties of DyBa2Cu2O7-d and its possible manufacture as thin film for power applications**
Department of Energy Conversion and Storage
Period: 01/09/2014 → 31/12/2017
Number of participants: 4
Phd Student:
Opata, Yuri Aparecido (Intern)
Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Yue, Zhao (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Science Without Borders, Brasi
Project: PhD

**In-situ 3D microstructure characterisation of solid oxide fuel cells using X-ray tomography methods**
Department of Energy Conversion and Storage
Period: 15/08/2014 → 13/12/2017
Number of participants: 7
Phd Student:
De Angelis, Salvatore (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Lauridsen, Erik Mejdal (Intern)
Main Supervisor:
Bowen, Jacob R. (Intern)
Examiner:
Andreassen, Jens Wenzel (Ekstern)
Carbone, Gerardina (Ekstern)
Chiu, Wilson K. S. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Activities:
Wilson K. S. Chiu
Gerardina Carbone

Publications:
Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography
Project: PhD

Robust HT-MEAs for Dynamic Operation under Smart Grid Conditions
Department of Electrical Engineering
Center for Electric Power and Energy
Energy resources, services and control
Department of Energy Conversion and Storage
Proton conductors
Period: 01/08/2014 → 01/08/2017
Number of participants: 3
Acronym: SmartMEA
Project participant:
Pensini, Alessandro (Intern)
Træholt, Chresten (Intern)

Project Manager, organisational:
Jensen, Jens Oluf (Intern)

Alkaline Electrolyser Cell
Department of Energy Conversion and Storage
Period: 01/08/2014 → 13/11/2017
Number of participants: 8
Phd Student:
Kraglund, Mikkel Rykaer (Intern)

Supervisor:
Aili, David (Intern)
Jensen, Jens Oluf (Intern)
Nikiforov, Aleksey Valerievich (Intern)
Main Supervisor:
Christensen, Erik (Intern)
Examiner:
Chatzichristodoulou, Christodoulos (Intern)
Sunde, Svein (Ekstern)
Therkildsen, Kasper Tipsmark (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Alkaline membrane water electrolysis with non-noble catalysts
Project: PhD

Roll-to-roll X-ray scattering and analysis
Department of Energy Conversion and Storage
Period: 01/08/2014 → 12/11/2018
Number of participants: 3
Phd Student:
Rossander, Lea Hildebrandt (Intern)
Solid oxide fuel cells for the renewable energy transition
Project nr 2014-1-12231 funded by Energinet.dk's ForskEL programme

Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 01/08/2014 → 31/03/2017
Number of participants: 1
electrochemistry, solid oxide fuel cells, SOFC
Acronym: SOFC4RET
Number of related Ph.D. students: 3
Project Manager, academic: Graves, Christopher R. (Intern)

CHEETAH FP7
CHEETAH - Cost-reduction through material optimisation and Higher EnErgy outpuT of solAr phOtovoltaic modules - joining Europe’s Research and Development efforts in support of its PV industry - is a combined collaborative project (CP) and coordination and support action (CSA) funded under the European Commission’s 7th Framework programme. CHEETAH’s aims to solve specific R&D issues in the EERA-PV Joint Program and to overcome fragmentation of European PV R&D in Europe and intensify the collaboration between R&D providers and industry to accelerate the industrialization of innovations.

Department of Energy Conversion and Storage
Functional organic materials
Period: 21/07/2014 → …
Number of participants: 1
Project participant: Beliat, Michail (Intern)

Green Production of Nanomaterials for Energy Conversion
Department of Energy Conversion and Storage
Period: 01/07/2014 → 30/09/2017
Number of participants: 8
Phd Student: Xu, Yu (Intern)
Supervisor: Hendriksen, Peter Vang (Intern)
Norby, Poul (Intern)
Simonsen, Søren Bredmose (Intern)
Main Supervisor: Kiebach, Wolff-Ragnar (Intern)
Examiner: Della Negra, Michela (Intern)
Aymonier, Cyril (Ekstern)
Lester, Edward Henry (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Relations
Publications:
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials Used in Energy Conversion Devices
Project: PhD

Electrochemical Reduction of CO2 to Sustainable Synthetic Fuels
Department of Energy Conversion and Storage
Period: 01/06/2014 → 20/09/2017
Number of participants: 6
Phd Student:
Bhowmik, Arghya (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tøjs (Intern)
Examiner:
Norby, Poul (Intern)
Skulason, Egill (Intern)
Studt, Felix (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Publications:
Design of oxide electrocatalysts for efficient conversion of CO2 into liquid fuels
Project: PhD

Electrospun functionalized nano-materials for ultra-compact de-NOX SCR system in naval shipping
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/05/2014 → 01/07/2016
Number of participants: 1
Acronym: BLUESHIP
Project ID: 605102
Project participant:
Esposito, Vincenzo (Intern)

Development of Proton Conductive membranes
Department of Energy Conversion and Storage
Period: 01/05/2014 → 09/07/2017
Number of participants: 7
Phd Student:
Kirkebæk, Andreas (Intern)
Supervisor:
Aili, David (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Li, Qingfeng (Intern)
Examiner:
Søndergaard, Roar R. (Intern)
Hjuler, Hans Aage (Intern)
Kerres, Jochen (Ekstern)

Financing sources
**Lifetime limiting effects in pre-commercial solid cell devices**

Department of Energy Conversion and Storage  
Period: 01/03/2014 → 21/06/2017  
Number of participants: 7  
Phd Student:  
Skafte, Theis Løye (Intern)  
Supervisor:  
Blennow Tullmar, Peter (Intern)  
Graves, Christopher R. (Intern)  
Main Supervisor:  
Hjelm, Johan (Intern)  
Examiner:  
Hauch, Anne (Intern)  
Lanzini, Andrea (Ekstern)  
Weber, André (Ekstern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Inks for fast processing of recyclable polymer solar cells**

Department of Energy Conversion and Storage  
Period: 15/01/2014 → 26/04/2017  
Number of participants: 5  
Phd Student:  
Benatto, Gisele Alves dos Reis (Intern)  
Main Supervisor:  
Krebs, Frederik C (Intern)  
Examiner:  
Andreasen, Jens Wenzel (Intern)  
Tanenbaum, David M. (Ekstern)  
Wang, Ergang (Ekstern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**Alliance for Imaging and Modelling of Energy Applications**

The CINEMA research alliance will develop unique 3D micro-structural characterization methods, which make it possible to investigate components under realistic conditions and in real time. This will enable correlation between performance and local changes in the microstructure.

Department of Energy Conversion and Storage  
Imaging and Structural Analysis  
Department of Physics  
Neutrons and X-rays for Materials Physics
Department of Wind Energy
Composites and Materials Mechanics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Scientific Computing
Mixed Conductors
Statistics and Data Analysis
University of Copenhagen
Northwestern University
University of Manchester
MaxLab
LM Wind Power
Haldor Topsoe AS
Xnovo Technology ApS
Rockwool International
Amminex Emissions Technology A/S
Period: 01/01/2014 → 31/12/2018
Number of participants: 26
Acronym: CINEMA
Project participant:
Mikkelsen, Lars Pilgaard (Intern)
Sørensen, Bent F. (Intern)
Bowen, Jacob R. (Intern)
Kuhn, Luise Theil (Intern)
Larsen, Rasmus (Intern)
Hansen, Per Christian (Intern)
Frandsen, Henrik Lund (Intern)
Gundlach, Carsten (Intern)
Dahl, Anders Bjørholm (Intern)
Yang, Shu-Yi (Intern)
Poulsen, Stefan Othmar (Intern)
Lyckegaard, Allan (Intern)
Lauridsen, Erik Mejdal (Intern)
Sørensen, Henning Osholm (Ekstern)
Project Manager, organisational:
Sørensen, Hanne (Intern)
Phd Student:
Jespersen, Kristine Munk (Intern)
Beil, Johannes (Ekstern)
Andersen, Michael (Intern)
Emerson, Monica Jane (Intern)
De Angelis, Salvatore (Intern)
Birkelund, Klaus (Ekstern)
Jacobsen, Hjalte Sylvest (Intern)
Chapelle, Lucie (Intern)
Supervisor:
Frandsen, Henrik Lund (Intern)
Project Manager, academic:
Andreasen, Jens Wenzel (Intern)
**Noble Metals Free Intermediate -Temperature Supported Liquid Phase Electrolyzer**

The strategic development of the NobleFree project is noble metal free intermediate-temperature (200-400 C) fuel cells and water electrolyser with the same characteristics as of the Nafion®, PBI and Aquivion™ systems. This goal will be achieved by use of alkaline metals dihydrogen phosphates as proton-conducting supported liquid phase electrolytes (SLPE). These electrolytes will be liquid immobilized on ceramic nano fibers, whiskers and powders. It has been discovered recently, that nickel, high-nickel alloys and austenitic stainless steels containing small amounts of Ti have high corrosion resistance in the molten alkali metals dihydrogen phosphates in the above mentioned temperature range. The NobleFree will start with the parallel development of electrolytes and nickel-based catalysts. The final stage of the project will be design and test of noble metal free intermediate temperature water electrolyser. Possibilities of use SLPE system as a fuel cell will be also studied.

Department of Energy Conversion and Storage

**Proton conductors**

Energy and Materials

Period: 01/01/2014 → …

Number of participants: 5

Acronym: Noble Free

Project participant:

Nikiforov, Aleksey Valerievich (Intern)

Bjerrum, Niels J. (Intern)

Petrushina, Irina (Intern)

Christensen, Erik (Intern)

Jensen, Jens Oluf (Intern)

**Sustainable Carbon Power**

SUCAP eller ("Grøn Kulkraft") handler om at fremstille ikke-fossilt kulstof til kombineret energilagring og CO2 fjernelse. Den centrale idé i SUCAP projektet er at konvertere kombinationen af elektrisk vedvarende energi og CO2 til kombinationen af kul og oxygen, altså til et lager af potentiel energi. Processen er absolut mulig rent kemisk, men ikke udviklet og afprøvet, idet den hidtil værre anset som ineffektiv og unødvendig til energilagring. Vi vil vise, at det er muligt og effektivt at lagre energi som kul. SUCAP handler primært om en reduktion af CO2 til kul, d.v.s. den fuldstændige omdannelse, men det er også muligt at foretage en partiel CO2 reduktion til f.eks. brændstofferne kulmonoxid (CO), metan (CH4), dimethyl ether (DME), methanol (CH3OH) og andre flydende energistoffer. Projektet har som opgave at udvikle metoder hertil og demonstrere gennemførelse af processen i praksis, samt at vurdere økonomien. Hvis effektiviteten kan blive rimelig, hvad vi tror, kan projektet få meget vidtrækkende betydning for samfundets energiforsyning.

Department of Chemistry
A wide range of research activities have arisen to support the Danish target of a 100% renewable energy system by 2050. Projects focused on individual aspects of the energy system, such as zero emissions buildings or intelligent power systems provide valuable insight, that facilitates flexibility throughout the energy system. CITIES will address this deficiency by establishing an integrated research centre covering all aspects of the energy system, including gas, power, district heating/cooling and biomass, and most importantly methods to forecast, control and optimize their interactions through the use of advanced ICT solutions.

The high densities of population, energy consumption, and energy and communications networks in cities offer the greatest potential for flexibility at the last cost, and the fact that cities account for 80% of global energy consumption and emissions [1] make the urban environment an ideal setting for energy systems integration research. CITIES will pioneer research into fully integrated city energy systems, building short-term operational models that feed longer term planning models, considering the spatiotemporal variations, interactions, dynamics and stochastics in the energy system. Low level models of system components will inform higher-level aggregate models employed in market and control framework design. The leading position of European academia and industry and the rapidly growing market for smart energy solutions indicates substantial scope for increased competitiveness and job creation within this field. CITIES will, in collaboration with its industrial and academic partners, conduct research with a view to developing tools for the implementation of integrated energy system solutions.

Center granted by Strategic Research Council.

To be a sustainable organisation.

Department of Applied Mathematics and Computer Science
Department of Civil Engineering
Department of Management Engineering
Department of Energy Conversion and Storage
Department of Informatics and Mathematical Modeling
Centre for IT-Intelligent Energy Systems in Cities

Aalborg University
Period: 01/01/2014 → 31/12/2019
Number of participants: 8
Strategic
Acronym: CITIES
Number of related Ph.D. students: 12
Project participant:
Madsen, Henrik (Intern)
Heller, Alfred (Intern)
Nielsen, Per Sieverts (Intern)
Pedersen, Allan Schröder (Intern)
Rode, Carsten (Intern)
Pinson, Pierre (Intern)
Jørgensen, John Bagterp (Intern)
Project Manager, organisational:
Herrmann, Ivan Tengbjerg (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Energy Programme
Relations
Activities:
Blockchain Summer School 2017
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
CITIES Annual Conference
3rd International Workshop on Design in Civil and Environmental Engineering
Executive Development Programme with Technical University of Denmark
12th International SDEWES Conference
Energy Supply Modelling in Cities: Illustrated Using Data from the Danish Municipality of Sønderborg
Energy Supply Modelling in Cities: Illustrated Using Data from the Case of Sønderborg
Big Data som værktøj til at styre byens energi
The 40th International IAEE Conference
Big Data as a tool for controlling the cities energy: Data aspects and data management
30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Status and Results of Energy Supply Modelling in CITIES: Illustrated using Data from the Case of Sønderborg

Publications:
Model Identification for Control of Display Units in Supermarket Refrigeration Systems

Center for Thermoelectric Energy Conversion
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2014 → 31/12/2018
Number of participants: 1
Acronym: CTEC
Working partner:
Van Nong, Ngo (Intern)

Project

Elektrode Kinetics and Gas Conversion in Solid Oxide Cells
Department of Energy Conversion and Storage
Period: 01/01/2014 → 20/04/2016
Number of participants: 7
Phd Student:
Njodzefon, Jean-Claude (Intern)
Supervisor:
Graves, Christopher R. (Intern)
Weber, André (Ekstern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Hauch, Anne (Intern)
Krügel, Albert (Ekstern)
Scheffold, Josef (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finsieret virksomhed

Relations
Publications:
Electrode Kinetics and Gas Conversion in Solid Oxide Cells
Project: PhD
**Elektrokatalyse og Katalysatorer til Oxygenreduktion i Polymer Brændselsceller**

**Department of Energy Conversion and Storage**

**Period:** 01/01/2014 → 17/05/2017  
**Number of participants:** 7  
**Phd Student:**  
Zhong, Lijie (Intern)  
**Supervisor:**  
Cleemann, Lars Nilausen (Intern)  
Jensen, Jens Oluf (Intern)  
**Main Supervisor:**  
Li, Qingfeng (Intern)  
**Examiner:**  
Bjerrum, Niels J. (Intern)  
Steenberg, Thomas (Intern)  
Steenberg, Thomas (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering

**Relations**

**Publications:**

- Graphitic Layer Encapsulated Iron Based Non-precious Catalysts for the Oxygen Reduction Reaction

**Materials for Energy Production**

**Department of Energy Conversion and Storage**

**Period:** 01/01/2014 → 26/04/2017  
**Number of participants:** 5  
**Phd Student:**  
Heckler, Ilona Maria (Intern)  
**Main Supervisor:**  
Bundgaard, Eva (Intern)  
**Examiner:**  
Andreassen, Jens Wenzel (Intern)  
Tanenbaum, David M. (Ekstern)  
Wang, Ergang (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering

**Relations**

**Publications:**

- Polymer materials for roll coated solar cells: strategies tom improve performance and stability

**Nano-carbons for versatile power supply modules**

NanoCaTe, a project co-financed by the European Commission, is focused on innovative flexible thermoelectric materials, based on standard and modified nanocarbon materials like graphene or carbon nanotubes. Twelve partners from Austria, Denmark, Finland, Germany, and Spain develop materials for thermoelectric energy harvesting and energy storage for manifold applications like pulsed sensors or mobile electronic devices. The integration of the developed materials into harvester and storage devices is a further step to characterize the performance of the innovative materials. Finally, a demonstrator consisting of harvester, storage and energy management represents a self-sustaining, universally usable, and maintenance-free power supply. The project strengthens the position of Europe in the field of thermoelectric and storage materials by developing devices with increased lifetime produced by cost-efficient technologies and therefore contributing to a further promotion of cleaner energy technologies.
For detailed information visit http://nanocate.eu/

Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/12/2013 → 30/09/2017
Number of participants: 1

NanoCaTe
Project Manager, academic:
Van Nong, Ngo (Intern)

Financing sources
Source: Public research council
Name of research programme: 7th Framework Programme for Research and Technological Development
Amount: 4,900,000.00 Euro

Organic based photovoltaics with morphological control
Department of Energy Conversion and Storage
Period: 01/10/2013 → 30/06/2015
Number of participants: 3
Phd Student:
Zawacka, Natalia Klaudia (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Jørgensen, Mikkel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Active Cooling of a Down Hole Well Tractor
Department of Energy Conversion and Storage
Period: 01/09/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Soprani, Stefano (Intern)
Supervisor:
Bahl, Christian (Intern)
Nesgaard, Carsten (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Van Nong, Ngo (Intern)
Veje, Christian T. (Ekstern)
Verda, Vittorio (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU

Relations
Publications:
Active cooling of a down hole well tractor
Project: PhD

Computational Design of Electrocatalysts for Sustainable Production of Synthetic Fuels
Department of Energy Conversion and Storage
Period: 01/09/2013 → 25/01/2017
Number of participants: 6
Phd Student:
Christensen, Rune (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Stephens, Ifan (Intern)
Reuter, Karsten (Ekstern)
Rossmeisl, Jan (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

**Relations**
Publications:
Error Mitigation in Computational Design of Sustainable Energy Materials
Project: PhD

**Design and testing of high performance regenerators**
Department of Energy Conversion and Storage
Period: 15/08/2013 → 14/12/2016
Number of participants: 7
Phd Student:
Lei, Tian (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Nielsen, Kaspar Kirstein (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Hattel, Jesper Henri (Intern)
Barbosa Jr., Jader R. (Ekstern)
Furberg, Richard (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Publications:
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow
Project: PhD

**High performance Magnetocaloric Materials**
Department of Energy Conversion and Storage
Period: 01/08/2013 → 30/09/2016
Number of participants: 7
Phd Student:
Neves Bez, Henrique (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Smith, Anders (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Bohr, Jakob (Intern)
Lo Bue, Martino (Ekstern)
Planes, Antoni (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Magnetocaloric materials and first order phase transitions
Project: PhD

Computational Investigations of transport mechanisms across battery interfaces
Department of Energy Conversion and Storage
Period: 01/07/2013 → 16/11/2016
Number of participants: 6
Phd Student:
Loftager, Simon (Intern)
Supervisor:
Garcia-Lastra, Juan Maria (Ekstern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Hjelm, Johan (Intern)
Khalifah, Peter (Ekstern)
Rossmeisl, Jan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Exploring Electronic Properties in All-oxide Heterostructures
Department of Energy Conversion and Storage
Period: 01/07/2013 → 13/11/2017
Number of participants: 7
Phd Student:
Christensen, Dennis Valbjørn (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Smith, Anders (Intern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Nygård, Jesper (Ekstern)
Eom, Chang-Beom (Ekstern)
Granozio, Fabio Miletto (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Mixed Rare Earth-Fe-B sintered magnets
Department of Energy Conversion and Storage
Period: 15/06/2013 → 06/04/2017
Number of participants: 7
Phd Student:
Xia, Manlong (Intern)
Supervisor:
Abrahamsen, Asger Bech (Intern)
Pryds, Nini (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Grivel, Jean-Claude (Intern)
Christensen, Mogens (Ekstern)
Paturi, Petriina (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Cost Effective Regenerative Metal Hydride Air Cell
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Period: 01/06/2013 → 01/06/2014
Number of participants: 1
Metal Hydride Air Cell
Acronym: CERMAC
Project participant:
Blanchard, Didier (Intern)

Optimised Hybrid Magnets
Department of Energy Conversion and Storage
Period: 01/06/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Insinga, Andrea Roberto (Intern)
Supervisor:
Björk, Rasmus (Intern)
Smith, Anders (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Beleggia, Marco (Intern)
Jensen, Bogi Bech (Intern)
Lomonova, Elena A. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Optimising Magnetostatic Assemblies
Project: PhD

Performance and lifetime limiting effects in Li-ion batteries
Department of Energy Conversion and Storage
Period: 01/06/2013 → 20/09/2016
Number of participants: 8
Phd Student:
Scipioni, Roberto (Intern)
Supervisor:
Hjelm, Johan (Intern)
Norby, Poul (Intern)
Main Supervisor:
Jensen, Søren Højgaard (Intern)
Examiner:
Bowen, Jacob R. (Intern)
Lindbergh, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Relations
Publications:
Performance and Lifetime Limiting Effects in Li-ion Batteries
Project: PhD

Mobility and Interfacial Effects under Degradation of Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 15/05/2013 → 16/06/2016
Number of participants: 6
Phd Student:
Corazza, Michael (Intern)
Supervisor:
Gevorgyan, Suren (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Project: PhD

Materials for Energy Production
Department of Energy Conversion and Storage
Period: 01/05/2013 → 16/06/2016
Number of participants: 5
Phd Student:
Livi, Francesco (Intern)
Main Supervisor:
Bundgaard, Eva (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed

Relations
Publications:
Conjugated Polymers for Energy Production
Project: PhD

HT PEMFC Durability and Lifetime
Department of Energy Conversion and Storage
Period: 01/04/2013 → 30/06/2016
Number of participants: 7
Phd Student:
Søndergaard, Tonny (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)
Examiner:
Petrushina, Irina (Intern)
Bajo, Justo Lobato (Ekstern)
Grahl-Madsen, Laila (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Mobility and Interfacial Effects under Degradation of Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 01/04/2013 → 16/06/2016
Number of participants: 5
Phd Student:
Roth, Bérenger (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Operational stability of large scale OPV modules: interfaces, materials selection and stack design
Project: PhD

Quantum and field effects of oxide heterostructures
Department of Energy Conversion and Storage
Period: 01/03/2013 → 30/09/2016
Number of participants: 7
Phd Student:
Trier, Felix (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Jespersen, Thomas Sand (Ekstern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Gabay, Marc (Ekstern)
Granizio, Fabio Miletto (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret

**Relations**
Publications:
Quantum and field effects of oxide heterostructures
Project: PhD

**Powerpipe hybrid solar panel**
A solar collector panel both producing electricity and heat will be developed and tested.

Department of Civil Engineering
Section for Building Physics and Services
Department of Energy Conversion and Storage
PowerPipe ApS
Batec Solvarme A/S
LOKE Lolland Energi
Period: 01/01/2013 → 30/06/2014
Number of participants: 3
Solar collector, Hybrid, Electricity, Heat
Project participant:
Furbo, Simon (Intern)
Fan, Jianhua (Intern)
Perers, Bengt (Intern)

**Financing sources**
Source: Forskningsprojekter - Miljø- og Energimisteriet
Name of research programme: EUDP programme
Amount: 489,600.00 Danish Kroner
Year of approval: 2012

**SMARTONICS FP7**
The target of the Smartonics project is the development of Pilot lines that will combine smart technologies with smart nanomaterials for the precision synthesis of Organic Electronic (OE) devices

Department of Energy Conversion and Storage
Functional organic materials
Period: 01/01/2013 → 01/08/2014
Number of participants: 1
Project participant:
Beliatis, Michail (Intern)

**Project**
AC superconducting wires

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2013 → 31/12/2013
Number of participants: 1
Superconductor, Coated conductor, Energy loss
Project participant:
Wulff, Anders Christian (Intern)

In-situ Neutron Imaging of Solid Oxide Fuel Cells

Department of Energy Conversion and Storage
Period: 01/01/2013 → 20/04/2016
Number of participants: 7
Phd Student:
Makowska, Małgorzata Grazyna (Intern)
Supervisor:
Lauridsen, Erik Mejdal (Intern)
Strobl, Markus (Ekstern)
Main Supervisor:
Kuhn, Luise Theil (Intern)
Examiner:
Hauch, Anne (Intern)
Grünzweig, Christian (Ekstern)
Hall, Stephen A. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Investigation of performance and lifetime limiting effects in Li-air battery cells

Department of Energy Conversion and Storage
Period: 01/12/2012 → 22/02/2016
Number of participants: 6
Phd Student:
Knudsen, Kristian Bastholm (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Hagen, Anke (Intern)
Adelhelm, Philipp (Ekstern)
Edström, Ester Kristina (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Alkali Metal-O2 Batteries. Performance and Lifetime Limiting Effects
Project: PhD
Management of Lithium-air batteries - safety, reliability and performance
Department of Energy Conversion and Storage
Period: 01/12/2012 → 20/04/2016
Number of participants: 7
Phd Student:
Christensen, Andreas Elkjær (Intern)
Supervisor:
Larsen, Esben (Intern)
Vestin, Karl (Ekstern)
Main Supervisor:
Norby, Poul (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Monroe, Charles William (Ekstern)
Møller, Per Jørgensen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Shaping our Energy Future with Electrospinning
Hans Christian Ørsted Postdoc Fellowship
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 15/10/2012 → 14/10/2014
Number of participants: 1
Project applicant:
Zhang, Wenjing (Angela) (Intern)

Oxygen Membranes for Biomass Gasification and Cement Industry
Department of Energy Conversion and Storage
Period: 01/09/2012 → 27/01/2016
Number of participants: 6
Phd Student:
Cheng, Shiyang (Intern)
Supervisor:
Kaiser, Andreas (Intern)
Main Supervisor:
Hendriksen, Peter Vang (Intern)
Examiner:
Kammer Hansen, Kent (Intern)
Guillon, Oliver (Ekstern)
Yu, Ji Haeng (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Preparation and characterization of cathode materials for lithium-oxygen batteries
Department of Energy Conversion and Storage
Period: 15/08/2012 → 20/09/2016
Number of participants: 6
Phd Student: Storm, Mie Møller (Intern)
Supervisor: Luntz, Alan (Ekstern)
Main Supervisor: Norby, Poul (Intern)
Examiner: Blanchard, Didier (Intern)
Choi, Jang Wook (Ekstern)
Nørgaard, Kasper (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Preparation and Characterization of Cathode Materials for Lithium-Oxygen Batteries
Project: PhD

Towards Smart Grid Ready SOFC
Department of Energy Conversion and Storage
Applied Electrochemistry
IRD Fuel Cells A/S
Topsoe Fuel Cell
Period: 01/08/2012 → 31/07/2014
Number of participants: 1
solid oxide fuel cells, smart grid, reformate gas, electrochemistry, durability, load cycles, stacks
Project Coordinator: Hjelm, Johan (Intern)

Computational analysis and design of new materials for lithium-air batteries
Department of Energy Conversion and Storage
Period: 01/08/2012 → 02/12/2015
Number of participants: 7
Phd Student: Mekonnen, Yedifana Setarge (Intern)
Supervisor: Garcia-Lastra, Juan Maria (Ekstern)
Hummelshøj, Jens Strabo (Intern)
Main Supervisor: Vegge, Tejs (Intern)
Examiner: Blanchard, Didier (Intern)
Rossmeisl, Jan (Intern)
Siegel, Donald Jason (Intern)

Pressurized HT PEM Cells for H2/O2 operation
Department of Energy Conversion and Storage
Period: 01/08/2012 → 30/09/2015
Number of participants: 7
Phd Student:
Søndergaard, Stine (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Petrushina, Irina (Intern)
Schmidt, Thomas Justus (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Anion Conducting Polymer Membranes for Hydrogen Production Through Alkaline Water Electrolysis
Department of Energy Conversion and Storage
Proton conductors
Period: 01/07/2012 → 30/06/2014
Number of participants: 1
Acronym: AlkaPEM
Project participant:
Aili, David (Intern)

Miljøvenlige, organiske solceller med kontrolleret nanostruktur, baseret på partikler i vandig dispersion
Department of Energy Conversion and Storage
Period: 01/06/2012 → 30/09/2015
Number of participants: 6
Phd Student:
Pedersen, Emil Bøje Lind (Intern)
Supervisor:
Aanaes, Henrik (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Müller, Christian (Ekstern)
Stingelin-Stutzmann, Natalie (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Hybrid metal-graphene nanostructured materials for innovative plasmonic electrodes
Department of Energy Conversion and Storage
Functional organic materials
Period: 01/03/2012 → 01/03/2014
Number of participants: 1
Acronym: UK EPSRC Postdoctoral Prize Fellowship
Project participant:
Beliatis, Michail (Intern)
**Direct conversion of carbon to electricity in a hybrid solid oxide fuel cell**

Department of Energy Conversion and Storage  
Period: 01/03/2012 → 03/06/2015  
Number of participants: 6  
Phd Student:  
Deleebeeck, Lisa (Intern)  
Supervisor:  
Mogensen, Mogens Bjerg (Intern)  
Main Supervisor:  
Kammer Hansen, Kent (Intern)  
Examiner:  
Hagen, Anke (Intern)  
Lagergren, Carina (Ekstern)  
Skou, Eivind Morten (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden EU-finansiering  
Project: PhD  

**Electrolyte and electrocatalysts combinations suitable for CO2 reduction and O2 evolution**

Department of Energy Conversion and Storage  
Period: 01/03/2012 → 02/09/2015  
Number of participants: 7  
Phd Student:  
Vico, Federica (Intern)  
Supervisor:  
Chatzichristodoulou, Christodoulos (Intern)  
Holtappels, Peter (Intern)  
Main Supervisor:  
Mogensen, Mogens Bjerg (Intern)  
Examiner:  
Bonanos, Nikolaos (Intern)  
Fabbri, Emiliana (Ekstern)  
Sunde, Svein (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  

**Relations**  
Publications:  
Searching for electrolytes and electrodes for CO2 reduction below 300 °C  
Project: PhD  

**Fabrication of Green Hydrocarbon Fuels via Capture and Electrolysis of CO2**

Department of Energy Conversion and Storage  
Period: 01/03/2012 → 13/05/2015  
Number of participants: 7  
Phd Student:  
Ebbehøj, Søren Lyng (Intern)  
Supervisor:  
Jensen, Søren Højgaard (Intern)  
Risager, Anders (Intern)  
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Hendriksen, Peter Vang (Intern)
Hansen, John Bøgild (Ekstern)
Hartvigsen, Joseph J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Integration of CO₂ air capture and solid oxide electrolysis for methane production
Project: PhD

Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery
Department of Energy Conversion and Storage
Period: 01/02/2012 → 02/12/2015
Number of participants: 7
Phd Student:
Pham, Hoang Ngan (Intern)
Supervisor:
Linderoth, Søren (Intern)
Nong, Ngo Van (Ekstern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Ramousse, Severine (Intern)
Eklund, Per (Ekstern)
Roch, Aljoscha (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

A Novel Thermoelectric Power Generator
The overall aim of this project is to demonstrate a cost-effective, mass-producible, and environmentally friendly technology for producing a novel thermoelectric generator, which overcomes the drawbacks typically found in the conventional technology. This type of thermal-to-electrical generating technology has broad applications ranging from a few mW up to kW devices. In order to achieve this goal, a thermoelectric module using an inexpensive ceramic forming process (tape casting) will be made during this project.

Thermo Ceramics
Electrofunctional materials

Department of Energy Conversion and Storage
Period: 01/01/2012 → 31/05/2012
Number of participants: 1
Project Coordinator:
Van Nong, Ngo (Intern)

Development of novel electrode-catalyst materials for Li-air battery cathodes
Department of Energy Conversion and Storage
Period: 01/01/2012 → 01/07/2015
Number of participants: 7
Phd Student:
Heijberg, Jonathan (Intern)
High-efficiency, low-cost electrode surfaces for next generation alkaline electrolysis

Department of Energy Conversion and Storage

Proton conductors

Energy and Materials

Department of Chemistry

Department of Chemistry

Period: 14/12/2011 → 12/12/2014

Number of participants: 3

Alkaline Electrolysis, Water splitting, Electrodes, Sustainable Energy

Project ID: J.nr. 068-2011-1

Project participant:

Nikiforov, Aleksey Valerievich (Intern)

Jensen, Jens Oluf (Intern)

Bjerrum, Niels J. (Intern)

Hydrogen from RES: pressurised alkaline electrolyser with high efficiency

The project RESelyser develops high pressure, highly efficient, low cost alkaline water electrolysers that can be integrated with renewable energy power sources (RES) using an advanced membrane concept, highly efficient electrodes and a new cell concept. A new concept with a three electrolyte loop system will be developed demonstrating even higher performance than conventional two electrolyte loop systems. This three electrolyte loop system will use a new separator membrane with internal electrolyte circulation and an adapted cell to improve mass transfer, especially gas evacuation. Intermittent and varying load operation connected to an RES will be addressed by improved electrode stability and a cell concept for increasing the gas purity of hydrogen and oxygen especially at low power as well as by a system concept. Electrolysers up to 30 kW with 6 Nm^3/h hydrogen production will be realized in the project. The primary pressure of the electrolyser will be above 25 bar (without the use of a compressor) to reduce the power loss for hydrogen compression to a minimum. All components of the system will be analyzed for their costs and developed to reduce the system price such that hydrogen can be produced at 3000 €/(Nm^3/h). An extrapolation to a primary electrolyser pressure of 100-150 bar is considered.

Department of Energy Conversion and Storage

Imaging and Structural Analysis

Fuel Cells and Solid State Chemistry Division

Microstructures and Interfaces

Deutsches Zentrum Für Luft- und Raumfahrt

Flemish Institute for Technological Research

Hydrogenics Europe NV

Period: 01/11/2011 → 30/04/2015

Number of participants: 3
Alkaline Electrolysis, Hydrogen
Acronym: RESelyser
Project ID: 48099
Project participant:
Jørgensen, Peter Stanley (Intern)
Bentzen, Janet Jonna (Intern)
Project Manager, academic:
Bowen, Jacob R. (Intern)

Financing sources
Source: EU research programme (public)
Name of research programme: FCH JU
Amount: 97,548.00 Euro
Year of approval: 2011

Relations
Activities:
SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
18th International Microscopy Congress
Publications:
RES Hydrogen: efficient pressurised alkaline electrolyser
Selected hydrogen production activities at the Institute of Technical Thermodynamics of DLR focused on the electrodes and stack design

Solar Hydrogen Fuel Production Station
Department of Energy Conversion and Storage
Functional organic materials
Period: 31/10/2011 → 01/09/2012
Number of participants: 1
Acronym: UK Knowledge Transfer Account (KTA)
Project participant:
Beliatis, Michail (Intern)

Kinetic studies and Computational Fluid Dynamics (CFD) simulations to aid in the development of Tantalum coated extreme corrosion resistance welded plate heat exchangers (ECWP)
Department of Energy Conversion and Storage
Period: 01/10/2011 → 17/12/2014
Number of participants: 8
Phd Student:
Mugabi, James Atwoki (Intern)
Supervisor:
Christensen, Erik (Intern)
Eriksen, Søren (Intern)
Petrushina, Irina (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Li, Qingfeng (Intern)
Papatheodorou, George (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD
Modelling environmentally friendly materials for magnetic refrigeration

Department of Energy Conversion and Storage  
Period: 01/10/2011 → 17/12/2014  
Number of participants: 7  
Phd Student:  
von Moos, Lars (Intern)  
Supervisor:  
Engelbrecht, Kurt (Intern)  
Nielsen, Kaspar Kirstein (Intern)  
Main Supervisor:  
Bahl, Christian (Intern)  
Examiner:  
Abrahamsen, Asger Bech (Intern)  
Burriel, Ramón (Ekstern)  
Cohen, Lesley (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD  

Computational Design of New Materials for Ammonia Storage

Department of Energy Conversion and Storage  
Period: 15/09/2011 → 17/12/2014  
Number of participants: 6  
Phd Student:  
Jensen, Peter Bjerre (Intern)  
Supervisor:  
Quaade, Ulrich (Intern)  
Main Supervisor:  
Vegge, Tejs (Intern)  
Examiner:  
Rossmeisl, Jan (Intern)  
Bligaard, Thomas (Intern)  
Hammer, Bjørk (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet  
Project: PhD  

Fremsættelse og karakterisering af elektrolytter og elektroder til vandelektrolyse i temperaturområdet 200-400°C

Department of Energy Conversion and Storage  
Period: 15/09/2011 → 11/03/2015  
Number of participants: 8  
Phd Student:  
Prag, Carsten Brorson (Intern)  
Supervisor:  
Christensen, Erik (Intern)  
Petrushina, Irina (Intern)  
Li, Qingfeng (Intern)  
Main Supervisor:  
Bjerrum, Niels J. (Intern)  
Examiner:  
Berg, Rolf W. (Intern)  
Steenberg, Thomas (Intern)
Sunde, Svein (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

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**Fremstilling og karakterisering af materiale og komponenter til mellemliggende emperatur brænselsceller og vandelektrolyse**

Department of Energy Conversion and Storage
Period: 15/08/2011 → 26/11/2014
Number of participants: 8
Phd Student:
Jensen, Annemette Hindhede (Intern)
Supervisor:
Barner, Jens H. Von (Intern)
Christensen, Erik (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Petrushina, Irina (Intern)
Bouzek, Karel (Ekstern)
Steenberg, Thomas (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

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**Development and processing of p-type oxide thermoelectric materials**

Department of Energy Conversion and Storage
Period: 01/08/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Wu, NingYu (Intern)
Supervisor:
Nong, Ngo Van (Ekstern)
Pryds, Nini (Intern)
Main Supervisor:
Linderoth, Søren (Intern)
Examiner:
Bahl, Christian (Intern)
Balke, Benjamin (Ekstern)
Eklund, Per (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

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**Modeling of shape instabilities occurring during sintering**

Department of Energy Conversion and Storage
Period: 15/07/2011 → 30/09/2014
Number of participants: 7
Phd Student:
Tadesse Molla, Tesfaye (Intern)
Development and processing of n-type oxide thermoelectric materials
Department of Energy Conversion and Storage
Period: 01/07/2011 → 30/09/2014
Number of participants: 7
Phd Student:
Han, Li (Intern)
Supervisor:
Nong, Ngo Van (Ekstern)
Pryds, Nini (Intern)
Main Supervisor:
Linderoth, Søren (Intern)
Examiner:
Kaiser, Andreas (Intern)
Palmqvist, Anders (Ekstern)
Weidenkaff, Anke (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of functionally graded thermoelectric materials based on optimal average figure-of-merit
Department of Energy Conversion and Storage
Period: 01/06/2011 → 26/11/2014
Number of participants: 5
Phd Student:
Le, Thanh Hung (Intern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
Gelbstein, Yaniv (Ekstern)
Rosendahl, Lasse (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Experimental tape casting of multilayer for flue gas purification
Department of Energy Conversion and Storage
Experimental Extrusion of Tubular Multilayer Materials for Oxygen Membranes

Department of Energy Conversion and Storage
Period: 01/05/2011 → 17/12/2014
Number of participants: 8
Phd Student:
Kothanda Ramachandran, Dhavanesan (Intern)
Supervisor:
Clemens, Frank J. (Ekstern)
Glasscock, Julie (Intern)
Segaard, Martin (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)
Examiner:
Grivel, Jean-Claude (Intern)
Akhtar, Farid (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Inorganic Proton Conducting Materials

Department of Energy Conversion and Storage
Period: 15/04/2011 → 24/09/2014
Number of participants: 6
Phd Student:
Anfimova, Tatiana (Intern)
Supervisor:
Bjerrum, Niels J. (Intern)
Main Supervisor:
Li, Qingfeng (Intern)
Examiner:
Bonanos, Nikolaos (Intern)
Jensen, Torben René (Intern)
Norby, Truls (Ekstern)

Financing sources
Source: Internal funding (public)
**Experimental Tape Casting of Adjacently Graded Materials for Magnetic Refrigeration**

Department of Energy Conversion and Storage  
Period: 01/04/2011 → 26/11/2014  
Number of participants: 8  
Phd Student:  
Bulatova, Regina (Intern)  
Supervisor:  
Andersen, Kjeld Bahm (Intern)  
Della Negra, Michela (Intern)  
Kaiser, Andreas (Intern)  
Main Supervisor:  
Bahl, Christian (Intern)  
Examiner:  
Agersted, Karsten (Ekstern)  
Ringgaard, Erling (Intern)  
Roosen, Andreas (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**SOFC Stack Diagnostics**

Department of Energy Conversion and Storage  
Period: 01/04/2011 → 04/02/2015  
Number of participants: 7  
Phd Student:  
Mosbæk, Rasmus Rode (Intern)  
Supervisor:  
Barfod, Rasmus Gottrup (Intern)  
Hendriksen, Peter Vang (Intern)  
Main Supervisor:  
Hjelm, Johan (Intern)  
Examiner:  
Nielsen, Jimmi (Intern)  
Haart, L. G. J. de (Ekstern)  
Weber, André (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD

**Adiabatic Liquid Piston Compressed Air Energy Storage**

Traditional Compressed Air Energy Storage (CAES) is seen as one of the most cost effective technologies for the bulk energy storage in the future flexible grid. The project will investigate the possible lift of the round trip efficiency by the introduction of Adiabatic Liquid Piston CAES (ALP-CAES) which is expected to be highly competitive.

Department of Mechanical Engineering  
Energy Engineering  
Thermal Energy  
Risø National Laboratory for Sustainable Energy  
Secretariat, IT
Medium Temperature Water Electrolysis

Hydrogen has the potential to provide a reliable, secure and clean source of power. Water offers a practical way of hydrogen production in association with renewable energy sources. The main challenges for water electrolysers are high cost, low efficiency and insufficient lifetime. The strategy of MEDLYS to address these issues is to develop novel materials and technologies for a medium temperature steam electrolyser operating at 200-400°C. The temperature range is optimal for 1) improving thermodynamics and kinetics of the process, 2) potentially replacing noble metal based catalysts with cost-effective alternatives, 3) allowing for a wide selection of construction materials from metals, ceramics and thermal plastics for conducting, insulating or sealing purposes and 4) maintaining long-term durability. MEDLYS will start with development of fundamental materials including inorganic/composite proton conducting electrolyte, alternative catalysts and other construction (electrode substrate, current collector, and bipolar plate) materials. Based on the materials, electrolyser components will be manufactured and a lab-scale cell will be constructed for evaluation and concept-proof test. The proposal is based on the results from ongoing activities within DSF HyCycle Center by most of the consortium partners, who have expertise from materials science and technological know-how and strong intention to further exploit the achievements after the project. The fulfillment of MEDLYS objectives is believed to bring breakthroughs in the hydrogen production technology, which, in turn, would promote the renewable energy technologies on a national as well as an European and global level.
Petrushina, Irina (Intern)
Project Coordinator:
Bjerrum, Niels J. (Intern)
Project

Udvikling og karakterisering af avancerede Li-batterier

Department of Energy Conversion and Storage
Period: 01/03/2011 → 02/09/2015
Number of participants: 7
Phd Student:
Christiansen, Ane Sælland (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Norby, Poul (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Pedersen, Allan Schröder (Intern)
Dahl, Søren (Intern)
Dominko, Robert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

In situ characterisation of structure and transport in battery electrolytes and electrodes

Department of Energy Conversion and Storage
Period: 01/01/2011 → 26/02/2014
Number of participants: 7
Phd Student:
Sveinbjörnsson, Dadi Þorsteinn (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Norby, Poul (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Hjelm, Johan (Intern)
David, William Ian Fraser (Ekstern)
Sørby, Magnus H. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Globaliseringsmidler
Project: PhD

Polymer photovoltaics - Largecells - R2R-produced polymer solar cells

Department of Energy Conversion and Storage
Period: 01/01/2011 → 26/02/2014
Number of participants: 5
Phd Student:
Hösel, Markus (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Laursen, Bo Wegge (Intern)
Lianos, Panagiotis (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Investigation of the degradation of solid oxide cells applied for electrolysis
Department of Energy Conversion and Storage
Period: 15/12/2010 → 26/02/2014
Number of participants: 6
Phd Student:
Tao, Youkun (Intern)
Supervisor:
Ebbesen, Sune Dalgaard (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Nielsen, Jimmi (Intern)
Brisse, Annabelle (Ekstern)
Irvine, John T. S. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Use of Biomass derived fuels for SOFC´s effect of fuel impurities
Department of Energy Conversion and Storage
Period: 15/12/2010 → 15/04/2016
Number of participants: 3
Phd Student:
Johnson, Gregory (Intern)
Supervisor:
Hjalmarsson, Per (Intern)
Main Supervisor:
Hagen, Anke (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

OXIDE THERMOELECTRICS FOR EFFECTIVE POWER GENERATION FROM WASTE HEAT
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/12/2010 → …
Number of participants: 1
Acronym: OTE-POWER
Project Manager, academic:
Van Nong, Ngo (Intern)

Financing sources
Source: Public research council
Name of research programme: The Danish Council for Strategic Research DSF
Amount: 21,000,000.00 Danish Kroner
Project
Risk-benefit analyser af funktionelle fødevarer – Fokus på D-vitamin
National Food Institute
Division of Food Chemistry
Division of Toxicology and Risk Assessment
Department of Energy Conversion and Storage

Mixed Conductors
Period: 01/12/2010 → 30/11/2014
Number of participants: 4
Project participant:
Burild, Anders (Intern)
Poulsen, Morten (Intern)
Frandsen, Henrik Lund (Intern)
Project Manager, organisational:
Jakobsen, Jette (Intern)

Degradation of nanoparticle composite solar cells comprising both organic and inorganic materials
Department of Energy Conversion and Storage
Period: 01/10/2010 → 13/05/2015
Number of participants: 6
Phd Student:
Andreasen, Birgitta (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Norman, Kion (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
A. Katz, Eugene (Ekstern)
Persson, Nils-Krister (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Nano-Structures of Organic-based photovoltaic Cells
Department of Energy Conversion and Storage
Period: 01/10/2010 → 18/12/2013
Number of participants: 7
Phd Student:
Böttiger, Arvid P.L. (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Yang, Xiaoniu (Ekstern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)
Examiner:
Bahl, Christian (Intern)
Moth-Poulsen, Kasper (Intern)
Persson, Nils-Krister (Ekstern)

Financing sources
Source: Internal funding (public)
Organic-based photovoltaic cells with morphology control

Department of Energy Conversion and Storage
Period: 01/10/2010 → 11/12/2013
Number of participants: 6
PhD Student:
Andersen, Thomas Rieks (Intern)
Supervisor:
Jørgensen, Mikkel (Intern)
Main Supervisor:
Bundgaard, Eva (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
Brabec, Christoph J. (Ekstern)
Lira-Cantu, Mónica (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Roll-to-roll adaptation of high efficiency organic-based photovoltaic cells

Department of Energy Conversion and Storage
Period: 01/10/2010 → 24/09/2014
Number of participants: 5
PhD Student:
Trofod, Thue (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Holtappels, Peter (Intern)
Moons, Ellen (Ekstern)
Thompson, Barry C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Large-area Organic and Hybrid Solar Cells

Department of Energy Conversion and Storage
Functional organic materials
Period: 01/09/2010 → 31/08/2014
Number of participants: 2
Acronym: Largecells
Project participant:
Krebs, Frederik C (Intern)
Søndergaard, Roar R. (Intern)

Relations
Publications:
Reversible degradation of inverted organic solar cells by concentrated sunlight
The use of polyurethane as encapsulating method for polymer solar cells—An inter laboratory study on outdoor stability in 8 countries
Interlaboratory outdoor stability studies of flexible roll-to-roll coated organic photovoltaic modules: Stability over 10,000 h
Roll-to-roll fabrication of polymer solar cells
Electrical and Photo-Induced Degradation of ZnO Layers in Organic Photovoltaics
Origin of size effect on efficiency of organic photovoltaics
Scalability and stability of very thin roll-to-roll processed large area indium-tin-oxide free polymer solar cell modules
The OE-A OPV demonstrator anno domini 2011
Solar cells with one-day energy payback for the factories of the future
Large-scale roll-to-roll photonic sintering of flexo printed silver nanoparticle electrodes
The ISOS-3 inter-laboratory collaboration focused on the stability of a variety of organic photovoltaic devices
Investigation of the degradation mechanisms of a variety of organic photovoltaic devices by combination of imaging techniques—the ISOS-3 inter-laboratory collaboration
Rapid flash annealing of thermally reactive copolymers in a roll-to-roll process for polymer solar cells
TOF-SIMS investigation of degradation pathways occurring in a variety of organic photovoltaic devices – the ISOS-3 inter-laboratory collaboration
Roll-to-Roll fabrication of large area functional organic materials
Polymer and organic solar cells viewed as thin film technologies: What it will take for them to become a success outside academia
On the stability of a variety of organic photovoltaic devices by IPCE and in situ IPCE analyses – the ISOS-3 inter-laboratory collaboration
Enhancing functionality of ZnO hole blocking layer in organic photovoltaics
Comparison of UV-Curing, Hotmelt, and Pressure Sensitive Adhesive as Roll-to-Roll Encapsulation Methods for Polymer Solar Cells
All solution processing of ITO-free organic solar cell modules directly on barrier foil
A rational method for developing and testing stable flexible indium- and vacuum-free multilayer tandem polymer solar cells comprising up to twelve roll processed layers
Economic assessment of solar electricity production from organic-based photovoltaic modules in a domestic environment
Stability of Polymer Solar Cells
Slot-die Coating of a High Performance Copolymer in a Readily Scalable Roll Process for Polymer Solar Cells
Comparison of Fast Roll-to-Roll Flexographic, Inkjet, Flatbed, and Rotary Screen Printing of Metal Back Electrodes for Polymer Solar Cells
Project

Nye typer af elektrokatalysatorer til elektrolyse- og brændselsceller
Department of Energy Conversion and Storage
Period: 01/09/2010 → 03/02/2014
Number of participants: 7
Phd Student:
Tomás García, Antonio Luis (Intern)
Supervisor:
Petrushina, Irina (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Berg, Rolf W. (Intern)
Shen, Pei Kang (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Theoretical investigations of novel materials for nitrogen fixation
Department of Energy Conversion and Storage
Period: 01/09/2010 → 11/12/2013
Number of participants: 6
Phd Student:
Howalt, Jakob Geelmuyden (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Holtappels, Peter (Intern)
Hammer, Bjørk (Intern)
Hellman, Anders (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Upscaling of Highly Flexible Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 01/09/2010 → 26/02/2014
Number of participants: 5
Phd Student:
Angmo, Dechan (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Holtappels, Peter (Intern)
Moons, Ellen (Ekstern)
Thompson, Barry C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Danish-Chinese Center for Organic based Photovoltaic Cells with Morphology Control
Department of Energy Conversion and Storage
Functional organic materials
Imaging and Structural Analysis
Period: 31/08/2010 → 31/08/2016
Number of participants: 12
Number of related Ph.D. students: 1
Project participant:
Oksbjerg, Birgit (Intern)
Trofod, Thue (Intern)
Bundgaard, Eva (Intern)
Andreasen, Jens Wenzel (Intern)
Norman, Kion (Intern)
Krebs, Frederik C (Intern)
Zawacka, Natalia Klaudia (Intern)
Jørgensen, Mikkel (Intern)
Angmo, Dechan (Intern)
Andersen, Thomas Rieks (Intern)
Bentzen, Janet Jonna (Intern)
Rossander, Lea Hildebrandt (Intern)


**Relations**

**Activities:**

High resolution ptychographic tomography of soft matter

**Publications:**

Spatial degradation mapping and componentwise degradation tracking in polymer-fullerene blends

Scalable, ambient atmosphere roll-to-roll manufacture of encapsulated large area, flexible organic tandem solar cell modules

In situ monitoring of structure formation in the active layer of polymer solar cells during roll-to-roll coating

The influence of additives on the morphology and stability of roll-to-roll processed polymer solar cells studied through ex situ and in situ X-ray scattering

Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging

All-Solution-Processed, Ambient Method for ITO-Free, Roll-Coated Tandem Polymer Solar Cells using Solution-Processed Metal Films

Medium area, flexible single and tandem junction solar cells based on roll coated semi-random copolymers

Roll-coating fabrication of flexible large area small molecule solar cells with power conversion efficiency exceeding 1%

Comparison of additive amount used in spin-coated and roll-coated organic solar cells

**Project**

**Højtemperatur PEM Brandselsceller og organiske brændsler**

Department of Energy Conversion and Storage

*Period: 01/08/2010 → 30/09/2014*

*Number of participants: 7*

Phd Student:

Vassiliev, Anton (Intern)

Supervisor:

Jensen, Jens Olf (Intern)

Li, Qingfeng (Intern)

Main Supervisor:

Bjerrum, Niels J. (Intern)

 Examiner:

Christensen, Erik (Intern)

Arico, Antonino Salvatore (Ekstern)

Kær, Søren Knudsen (Ekstern)

**Financing sources**

*Source: Internal funding (public)*

*Name of research programme: Institut stipendie (DTU) Samf.*

*Project: PhD*

**Indium-tin-oxide free roll-to-roll processed polymer solar cells**

Department of Energy Conversion and Storage

*Period: 01/08/2010 → 11/12/2013*

*Number of participants: 5*

Phd Student:

Dam, Henrik Friis (Intern)

Main Supervisor:

Krebs, Frederik C (Intern)

Examiner:

Brabec, Christoph J. (Ekstern)

Kuhn, Luise Theil (Intern)

Yu, Donghong (Ekstern)

**Financing sources**

*Source: Internal funding (public)*

*Name of research programme: Forskningsrådsfinansiering*

*Project: PhD*
Large Area Roll-to-roll processed photocatalytic films for solar energy conversion and storage

Department of Energy Conversion and Storage
Period: 01/08/2010 → 26/02/2014
Number of participants: 5
Phd Student:
Jensen, Jacob (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Laursen, Bo Wegge (Intern)
Lianos, Panagiotis (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development and application of a green Chemistry solution deposition technique for buffer layer coating on cue-textured metal substrates in view of further deposition of rare-earth based superconductors

Department of Energy Conversion and Storage
Period: 01/07/2010 → 26/02/2014
Number of participants: 5
Phd Student:
Pallewatta, Pallewatta G A P (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)
Examiner:
Kaiser, Andreas (Intern)
Rubesova, Katerina (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Development of a fluorine-free chemical solution deposition route for rare-earth cuprate superconducting tapes and its application to reel-to-reel

Department of Energy Conversion and Storage
Period: 01/07/2010 → 30/09/2013
Number of participants: 5
Phd Student:
Tang, Xiao (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)
Examiner:
Agersted, Karsten (Ekstern)
Augieri, Andrea (Ekstern)
Driessche, Isabel J. M. Van (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Durable and Robust SOFC
This 2-year project had as one of its’ overarching goals to improve durability and robustness of the Danish solid oxide fuel cells. The project focus was on cells and cell components suitable for SOFC operation in the temperature range 600 – 750 °C. The cells developed and/or studied in this project are intended for use within the CHP (Combined Heat and Power) market segment with stationary power plants in the range 1 – 250 kW e in mind. A significant part of this project was concerned with improved understanding of degradation and failure mechanisms.

Department of Energy Conversion and Storage
Applied Electrochemistry
IRD Fuel Cells A/S
Period: 01/07/2010 → 30/06/2012
Number of participants: 1
solid oxide fuel cells , electrochemistry, degradation, durability, lifetime limiting factors, porous electrode, functional ceramics, high temperature materials, hydrogen
Project Coordinator:
Hjelm, Johan (Intern)
Financing sources
Source: Public research programme (public)
Name of research programme: ForskEL (Energinet.dk)
Web address: http://www.forskel.dk
Amount: 11,000,000.00 Danish Kroner
Year of approval: 2010

Electrolytes for electrochemical N2 fixation cells
Department of Energy Conversion and Storage
Period: 15/05/2010 → 30/09/2013
Number of participants: 6
Phd Student:
Lapina, Alberto (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Vegge, Tejs (Intern)
Haart, L. G. J. de (Ekstern)
Irvine, John T. S. (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Low Temperature oxidation of hydrocarbons using an electrochemical reactor
Department of Energy Conversion and Storage
Period: 01/05/2010 → 19/08/2013
Number of participants: 6
Phd Student:
Ippolito, Davide (Intern)
Supervisor:
Christensen, Henrik (Ekstern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Bonanos, Nikolaos (Intern)
Marnellos, George E. (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Degradation mechanism of the LSCF Cathode
Department of Energy Conversion and Storage
Period: 15/04/2010 → 19/03/2013
Number of participants: 7
Phd Student:
Zhang, Weiwei (Intern)
Supervisor:
Barfod, Rasmus Gottrup (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Chen, Ming (Intern)
Examiner:
Hjelm, Johan (Intern)
Hallstedt, Bengt (Ekstern)
Markus, Torsten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Development of improved electrodes in high temperature PEM fuel cells
Department of Energy Conversion and Storage
Period: 15/03/2010 → 11/12/2013
Number of participants: 7
Phd Student:
Permyakova, Anastasia Aleksandrovna (Intern)
Supervisor:
Jensen, Jens Oluf (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Christensen, Erik (Intern)
Arenz, Matthias (Ekstern)
Bajo, Justo Lobato (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

BioSOFC - 3rd Generation Biomass Based Combined Heat and Power (CHP)
The aim of project is to investigate the combination of biomass gasification with SOFC in an efficient decentralized and flexible energy system for small scale combined heat and power production. The project work includes design, construction and long term operation of a gasifier-SOFC stack test set-up, analysis of performance and system analysis.
Department of Mechanical Engineering
Energy Engineering
Thermal Energy
Low Temperature NOx decomposition using an electrochemical Reactor

Department of Energy Conversion and Storage
Period: 01/03/2010 → 19/08/2013
Number of participants: 5
Phd Student: Shao, Jing (Intern)
Main Supervisor: Kammer Hansen, Kent (Intern)
Examiner: Hjelm, Johan (Intern)
Kustov, Arkadii (Intern)
Vernoux, Philippe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Test and Approval Center for Fuel Cell and Hydrogen Technologies: Phase I. Initiation

Department of Energy Conversion and Storage
Applied Electrochemistry
Danish Gas Technology Centre A/S
Period: 01/01/2010 → 30/06/2012
Number of participants: 1
Project participant: Hagen, Anke (Intern)

Relations
Publications:
Accelerated testing of solid oxide fuel cell stacks for micro combined heat and power application
Electrolytes for Synthesis of CO2-neutral Fuels

Department of Energy Conversion and Storage
Period: 01/01/2010 → 19/08/2013
Number of participants: 7
Phd Student:
Hallinder, Jonathan (Intern)
Supervisor:
Hagen, Anke (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Li, Qingfeng (Intern)
Grahl-Madsen, Laila (Ekstern)
Stimming, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Electrochemical Removal of NOx and Hydrocarbons

Department of Energy Conversion and Storage
Period: 01/12/2009 → 17/12/2014
Number of participants: 5
Phd Student:
Friedberg, Anja Zarah (Intern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Rasmussen, Søren Birk (Intern)
Tsiplakides, Dimitrios T. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Synthesis of new polymer materials for high efficiency photovoltaire cells

Department of Energy Conversion and Storage
Period: 01/10/2009 → 24/06/2013
Number of participants: 6
Phd Student:
Carlé, Jon Eggert (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Jørgensen, Mikkel (Intern)
Examiner:
Sommer-Larsen, Peter (Intern)
Christensen, Jørn B. (Ekstern)
R. Andersson, Mats (Ekstern)

Financing sources
Computational analysis of the interaction of water with materials for energy storage

Department of Energy Conversion and Storage
Period: 15/09/2009 → 19/03/2013
Number of participants: 6
Phd Student:
Lysgaard, Steen (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Hellman, Anders (Ekstern)
Jónsson, Hannes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Computational screening of new carbon-neutral energy materials

Department of Energy Conversion and Storage
Period: 15/09/2009 → 19/03/2013
Number of participants: 6
Phd Student:
Mýrdal, Jón Steinar Garðarsson (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Schietz, Jakob (Intern)
David, William Ian Fraser (Ekstern)
Ikeshoji, Tamio (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Development of long cube textured metal substrates suitable for reel-to-reel processing and applications under both ac and dc conditions

Department of Energy Conversion and Storage
Period: 01/09/2009 → 28/01/2013
Number of participants: 7
Phd Student:
Wulff, Anders Christian (Intern)
Supervisor:
Andersen, Niels Hessel (Intern)
Mishin, Oleg (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)
Examiner:
Juul Jensen, Dorte (Intern)
Glowacki, Bartek A. (Ekstern)
Holzapfel, Bernhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Nanostructered Ceramic Oxygen Sensors
Department of Energy Conversion and Storage
Period: 01/09/2009 → 17/12/2012
Number of participants: 6
Phd Student:
Hu, Qiang (Intern)
Supervisor:
Hansen, Karin Vels (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Holtappels, Peter (Intern)
Skou, Eivind Morten (Ekstern)
Wiemhöfer, Hans-Dieter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

New Electrolytes for CO2 Electrolysis Cells
Department of Energy Conversion and Storage
Period: 01/09/2009 → 19/03/2013
Number of participants: 7
Phd Student:
Mollerup, Pia Lolk (Intern)
Supervisor:
Bonanos, Nikolaos (Intern)
Tullmar, Peter Blennov (Ekstern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Jensen, Jens Oluf (Intern)
Friedrich, Kaspar Andreas (Ekstern)
Kiros, Yohannes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Lengthening the Lifetime ofR2R-produced Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 01/08/2009 → 24/06/2013
Number of participants: 5
Phd Student:
Madsen, Morten Vesterager (Intern)
Supervisor:
Krebs, Frederik C (Intern)
**High Performance polymer solar cells through rational characterization and design**

Department of Energy Conversion and Storage  
**Period:** 01/07/2009 → 19/10/2012  
**Number of participants:** 5  
**Phd Student:** Tromholt, Thomas (Intern)  
**Main Supervisor:** Krebs, Frederik C (Intern)  
**Examiner:** Norby, Poul (Intern)  
**Nelson, Jenny (Ekstern)  
**Rivaton, Agnès (Ekstern)**  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Programbevilling  
Project: PhD

**High Temperature AlkalineElectrolyser Cell**

Department of Energy Conversion and Storage  
**Period:** 15/05/2009 → 01/03/2013  
**Number of participants:** 7  
**Phd Student:** Allebrod, Frank (Intern)  
**Supervisor:** Ebbesen, Sune Dalgaard (Intern)  
**Hjelm, Johan (Intern)  
**Main Supervisor:** Mogensen, Mogens Bjerg (Intern)  
**Examiner:** Holtappels, Peter (Intern)  
**Skou, Eivind Morten (Ekstern)  
**Sunde, Svein (Ekstern)**  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Electrochemical Reduction of NOx**

Department of Energy Conversion and Storage  
**Period:** 01/05/2009 → 27/06/2012  
**Number of participants:** 5  
**Phd Student:** Traulsen, Marie Lund (Intern)  
**Main Supervisor:** Kammer Hansen, Kent (Intern)
A high performance ion transport membrane (HP-ITM)
In the project HP-ITM, ion transport membranes (ITM) have been developed and oxygen fluxes of more than 5 ml min$^{-1}$ cm$^{-2}$ have been demonstrated. The project also documents potential limitations of the current demonstration pieces regarding mechanical strength of the ceramic supports and chemical expansion of the ceria based membrane materials.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/04/2009 → 30/06/2010
Number of participants: 1
Acronym: HP-ITM
Number of related Ph.D. students: 1
Project participant:
Kaiser, Andreas (Intern)

Financing sources
Source: Public research council
Name of research programme: Proof of Concept for public research institutes
Amount: 966,439.04 Danish Kroner
Year of approval: 2007

Relations
Publications:
On the use of supported ceria membranes for oxyfuel process/syngas production
Oxygen permeation in thin, dense Ce0.9Gd0.1O 1.95- membranes II. experimental determination
Evaluation of thin film ceria membranes for syngas membrane reactors—Preparation, characterization and testing

Development of 3D EBSD for characterisation of solid oxide electrolysis cells in relation to performance and degradation
Department of Energy Conversion and Storage
Period: 01/04/2009 → 30/09/2015
Number of participants: 6
PhD Student:
Saowadee, Nath (Intern)
Supervisor:
Agersted, Karsten (Ekstern)
Main Supervisor:
Bowen, Jacob R. (Intern)
Examiner:
Lauridsen, Erik Mejdal (Intern)
Gholinia, Ali (Ekstern)
Ringgaard, Erling (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Privatist
Project: PhD

Fremstilling og synteseanvendelse af elektrolytisk fremstillet hydrogen
Cathodes for solid Oxide Fuel Cells Operating at 400 C

Anodes for SOFCs Operating at 400 degrees
Project: PhD

Computational methods for describing reaction rates at interfaces of energy materials
Department of Energy Conversion and Storage
Period: 01/12/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Maronsson, Jon Bergmann (Intern)
Supervisor:
Jonsson, Hannes (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Henkelman, Graeme (Ekstern)
Wahnström, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

3D Studies of Coarsening Kinetics of Individual Grains
Department of Energy Conversion and Storage
Period: 01/09/2008 → 29/03/2012
Number of participants: 6
Phd Student:
Poulsen, Stefan Othmar (Intern)
Supervisor:
Juul Jensen, Dorte (Intern)
Main Supervisor:
Lauridsen, Erik Mejdal (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Moelans, Nele (Ekstern)
Rollett, Anthony David (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Investigating the Stability of Electrode-electrolyte-interfaces
Department of Energy Conversion and Storage
Period: 01/02/2008 → 08/02/2012
Number of participants: 6
Phd Student:
Torres da Silva, Iris Maura (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Skaarup, Steen (Intern)
Skou, Eivind Morten (Ekstern)
Weber, André (Ekstern)
Innovative solid oxide electrolyser stacks for efficient and reliable hydrogen production

The RelHy project targets the development of novel or improved, low cost materials (and the associated manufacturing process) for their integration in efficient and durable components for the next generation of electrolyzers based on Solid Oxide Electrolysis Cells (SOEC). It is specifically tailored for 1) Optimisation of novel or improved cell, interconnect and sealing materials, 2) Achievement of innovative designs for SOE stacks to improve durability. As such, it is positioned as a bridge between currently good performing electrolysis cells and their efficient and reliable integration into advanced stacks to pave the way for the production of a new generation of electrolyzers. To achieve these goals, the RelHy project is based on the coupled development of instrumented single repeat units and stacks and of associated simulation tools (from cell to stack scale). This mixed experimental and simulation approach will be used on several batches of materials - to give specifications for novel or improved materials and evaluate them, where special attention is paid to material compatibility (between electrodes, electrolyte, coating, interconnects and sealing). - to propose innovative designs able to overcome the present limiting parameters and to increase stack reliability, durability and performance. These material and design innovations will be validated at laboratory scale on a 25-cell stack prototype and its competitiveness will be assessed. Since the project is centered on R&D activities, the RelHy multidisciplinary European consortium is merging expertise from two university laboratories and three research centres already recognised for material development and cell production, instrumentation and testing, and modelling (DTU-Risoe, Imperial College, ECN, EIFER and CEA) and also from a fuel cell stack manufacturer that can produce electrolyser stacks (TOFC) and from an energy company (HELION) that can specify the operation conditions and assess the competitiveness of the innovative electrolyser prototype and its potential integration. The main issue addressed in the project is the simultaneous achievement of both, lifetime (degradation close to 1% for 1000 hr on single repeat units at 800°C) and efficiency (0.03 to 0.04 gH2/cm2/hr, i.e. approximately 1 A/cm2 with water utilisation >60% and a stack efficiency > 90%). These operation points and degradation values will yield an efficiency of up to 80% (LHV) at the system level with >99% availability. Cost issues will also be addressed by considering cost effective materials and processes in order to meet the “non energy” 1€/kg H2 target.

Department of Energy Conversion and Storage

Applied Electrochemistry

Risø National Laboratory for Sustainable Energy

Fuel Cells and Solid State Chemistry Division

Electrochemical Evaluation

Electrochemistry

Period: 01/01/2008 → 31/12/2011
Number of participants: 3
High temperature electrolysis
Acronym: RelHy
Project participant:
Ebbesen, Sune Dalgaard (Intern)
Ehora, Ghislaine (Intern)
Project Manager, organisational:
Bowen, Jacob R. (Intern)

Financing sources

Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 4,733,454.00 Danish Kroner

Relations

Activities:
Microstructure characterisation of solid oxide electrolysis cells operated at high current density

Polymer Solar Cells for Solar Energy Conversion
DSF sagsnr.: 2104-07-0022, DTU projektnr.: 48010

Department of Energy Conversion and Storage

Functional organic materials
Period: 01/01/2008 → 31/12/2013
Number of participants: 1
Project Manager, academic:
Krebs, Frederik C (Intern)

Relations
Publications:

Solar Test Platform
Low band gap polymers for organic solar cells
Thermally reactive Thiazolo[5,4-d]thiazole based copolymers for high photochemical stability in polymer solar cells
Advanced Functional Polymers for Increasing the Stability of Organic Photovoltaics
Concentrated Light for Accelerated Photo Degradation of Polymer Materials
Non-destructive lateral mapping of the thickness of the photoactive layer in polymer-based solar cells
Aesthetically Pleasing Conjugated Polymer: Fullerene Blends for Blue-Green Solar Cells Via Roll-to-Roll Processing
Ambient fabrication of flexible and large-area organic light-emitting devices using slot-die coating
Application of optical coherence tomography (OCT) as a 3-dimensional imaging technique for roll-to-roll coated polymer solar cells
Comparative studies of photochemical cross-linking methods for stabilizing the bulk hetero-junction morphology in polymer solar cells
Enhancing functionality of ZnO hole blocking layer in organic photovoltaics
Exciton diffusion length in some thermocleavable polythiophenes by the surface photovoltage method
Influence of processing and intrinsic polymer parameters on photochemical stability of polythiophene thin films
Investigation of the degradation mechanisms of a variety of organic photovoltaic devices by combination of imaging techniques—the ISOS-3 inter-laboratory collaboration
Large-scale roll-to-roll photonic sintering of flexo printed silver nanoparticle electrodes
Low-temperature side-chain cleavage and decarboxylation of polythiophene esters by acid catalysis
New Low-Bandgap Materials with Good Stabilities and Efficiencies Comparable to P3HT in R2R-Coated Solar Cells
On the stability of a variety of organic photovoltaic devices by IPCE and in situ IPCE analyses – the ISOS-3 inter-laboratory collaboration
Photochemical stability of conjugated polymers, electron acceptors and blends for polymer solar cells resolved in terms of film thickness and absorbance
Roll-to-roll fabrication of polymer solar cells
Solar cells with one-day energy payback for the factories of the future
Stability of Polymer Solar Cells
The ISOS-3 inter-laboratory collaboration focused on the stability of a variety of organic photovoltaic devices
The use of polyurethane as encapsulating method for polymer solar cells—An inter laboratory study on outdoor stability in 8 countries
TOF-SIMS investigation of degradation pathways occurring in a variety of organic photovoltaic devices – the ISOS-3 inter-laboratory collaboration
A compact multi-chamber setup for degradation and lifetime studies of organic solar cells
A life cycle analysis of polymer solar cell modules prepared using roll-to-roll methods under ambient conditions
An inter-laboratory stability study of roll-to-roll coated flexible polymer solar modules
A self-calibrating led-based solar test platform
A solution process for inverted tandem solar cells
Consensus stability testing protocols for organic photovoltaic materials and devices
Degradation of semiconducting polymers by concentrated sunlight
Economic assessment of solar electricity production from organic-based photovoltaic modules in a domestic environment
Electrical and Photo-Induced Degradation of ZnO Layers in Organic Photovoltaics
Ellipsometry as a Nondestructive Depth Profiling Tool for Roll-to-Roll Manufactured Flexible Solar Cells
Fabrication of Polymer Solar Cells Using Aqueous Processing for All Layers Including the Metal Back Electrode
Fused thiophene/quinoxaline low band gap polymers for photovoltaic’s with increased photochemical stability
Life-cycle analysis of product integrated polymer solar cells
Origin of size effect on efficiency of organic photovoltaics
Oxygen- and water-induced degradation of an inverted polymer solar cell: the barrier effect
Photochemical stability and photovoltaic performance of low-band gap polymers based on dithiophene with different bridging atoms
Polymers for organic photovoltaics based on 1,5-bis(2-hexyldecyloxy)-naphthalene, thiophene, and benzothiadiazole
Business, market and intellectual property analysis of polymer solar cells
Water and oxygen induced degradation of small molecule organic solar cells
Roll-to-Roll Processing of Inverted Polymer Solar Cells using Hydrated Vanadium(V)Oxide as a PEDOT:PSS Replacement
Printed metal back electrodes for R2R fabricated polymer solar cells studied using the LBIC technique
Degradation Patterns in Water and Oxygen of an Inverted Polymer Solar Cell
Influence of the Annealing Temperature on the Photovoltaic Performance and Film Morphology Applying Novel Thermocleavable Materials
Low band gap polymers based on 1,4-dialkoxybenzene, thiophene, bithiophene donors and the benzothiadiazole acceptor
Low Band Gap Polymers for Roll-to-Roll Coated Polymer Solar Cells
Manufacture, integration and demonstration of polymer solar cells in a lamp for the Lighting Africa initiative
Photovoltaic Performance of Polymers Based on Dithienylthienopyrazines Bearing Thermocleavable Benzoate Esters
Product integration of compact roll-to-roll processed polymer solar cell modules: methods and manufacture using flexographic printing, slot-die coating and rotary screen printing
The effect of post-processing treatments on inflection points in current–voltage curves of roll-to-roll processed polymer photovoltaics
Thermo-cleaveable polymers: Materials with enhanced photochemical stability
The teraton challenge. A review of fixation and transformation of carbon dioxide
Ultra Fast and Parsimonious Materials Screening for Polymer Solar Cells Using Differentially Pumped Slot-Die Coating
Upscaling of polymer solar cell fabrication using full roll-to-roll processing
Using Light-Induced Thermocleavage in a Roll-to-Roll Process for Polymer Solar Cells
All solution roll-to-roll processed polymer solar cells free from indium-tin-oxide and vacuum coating steps
A roll-to-roll process to flexible polymer solar cells: model studies, manufacture and operational stability studies
A round robin study of flexible large-area roll-to-roll processed polymer solar cell modules
Fabrication and processing of polymer solar cells: A review of printing and coating techniques
"Hairy" Poly(3-hexylthiophene) Particles Prepared via Surface-Initiated Kumada Catalyst-Transfer Polycondensation
Investigation of optical spacer layers from solution based precursors for polymer solar cells using X-ray reflectometry
Pad printing as a film forming technique for polymer solar cells
Polymer solar cell modules prepared using roll-to-roll methods: Knife-over-edge coating, slot-die coating and screen printing
Roll-to-roll fabrication of monolithic large-area polymer solar cells free from indium-tin-oxide
Study of hybrid solar cells made of multilayer nanocrystalline titania and poly(3-octylthiophene) or poly-(3-(2-methylhex-2-yl)-oxy-carbonyldithiophene)
Thermocleavable Materials for Polymer Solar Cells with High Open Circuit Voltage-A Comparative Study
Thermo-cleaveable solvents for printing conjugated polymers: Application in polymer solar cells
Water-Induced Degradation of Polymer Solar Cells Studied by (H2O)-O-18 Labeling
Air stable polymer photovoltaics based on a process free from vacuum steps and fullerenes
All solution processed tandem polymer solar cells based on thermocleavable materials
An explanation for the high stability of polycarboxythiophenes in photovoltaic devices—A solid-state NMR dipolar recoupling study
Applicability of X-ray reflectometry to studies of polymer solar cell degradation
A setup for studying stability and degradation of polymer solar cells
A simple nanostructured polymer/ZnO hybrid solar cell - preparation and operation in air
Biodegradable polymer solar cells
Bulk heterojunctions based on native polythiophene
Thermocleavable Low Band Gap Polymers and Solar Cells Therefrom with Remarkable Stability toward Oxygen
Structural and chemical investigation of CdSe crystals deposited in a nanoporous sol–gel: Effect of chemistry and defects on photovoltaic properties
Analysis of the failure mechanism for a stable organic photovoltaic during 10 000 h of testing
The OE-A OPV demonstrator anno domini 2011
Ultra high open circuit voltage (>1 V) of poly-3-hexylthiophene based organic solar cells with concentrated light
Polymer Solar Cells – Non Toxic Processing and Stable Polymer Photovoltaic Materials
Stability and Degradation of Organic and Polymer Solar Cells
Polymeric solar cells; materials, design, manufacture
Polymer photovoltaics: A practical approach
Organic solar cells
Characterization and Reporting of OPV Device Lifetime
Concentrated Light for Organic Photovoltaics
Degradation of Polymer-Based OPV
Polymersolceller
The Different PV Technologies and How They Degrade
Introduction
Manufacture
Market Analysis
Materials and Processing
Patent Overview of OPVs
Stability and Characterization of Devices
Technology Potential and Outlook
Introduction
Lifetime and stability studies
Outlook
Processing and production of large modules
The polymer solar cell
Photovoltaics efficiency improvements
Energy efficient Solid State Lighting
Solar energy
Combined Characterization Techniques to Understand the Stability of a Variety of Organic Photovoltaic Devices - the
ISOS-3 inter- laboratory collaboration
Optical coherence tomography (OCT) as a 3-dimensional imaging technique for non-destructive testing of roll-to-roll
coated polymer solar cells
Edge sealing for low cost stability enhancement of roll-to-roll processed flexible polymer solar cell modules
Interlayer adhesion in roll-to-roll processed flexible inverted polymer solar cells
Quality control of roll-to-roll processed polymer solar modules by complementary imaging methods
Simple roll coater with variable coating and temperature control for printed polymer solar cells
Stability and degradation of organic photovoltaics fabricated, aged, and characterized by the ISOS 3 inter-laboratory
collaboration
Economical assessment of solar electricity from organic photovoltaic systems
Large area modules based on low band gap polymers
Polymer solar cells for solar energy conversion
Solar energy – new photovoltaic technologies
Improved adhesion of metal oxide layer
Improved electron transport layer
PROCESS OF ELECTRICAL CONNECTION OF PHOTOVOLTAIC DEVICES
Photovoltaic device
Air Stable Photovoltaic Device
Method of Testing Solar Cells
Method of Thermocleaving a Polymer Layer
Editorial for the special issue on ISOS-3 (Third International Summit on OPV Stability)
Video editorial for the special issue on ISOS-3 (3rd international summit on OPV stability)
Editorial for the special issue on EMRS-A
Editorial: Reporting solar cell efficiencies in Solar Energy Materials and Solar Cells
Solceller lavet af plast
Automatic Quantitative Image Analysis of 3D Micrographs
Department of Informatics and Mathematical Modeling
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Period: 01/03/2007 → 22/09/2010
Number of participants: 7
PhD Student:
Jørgensen, Peter Stanley (Intern)
Supervisor:
Bowen, Jacob R. (Intern)
Hansen, Karin Vels (Intern)
Main Supervisor:
Larsen, Rasmus (Intern)
Examiner:
Bærentzen, Jakob Andreas (Intern)
Barnett, Scott (Intern)
Østergaard, Lasse Riis (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of software for the analysis of positron lifetime spectra
Development and world wide sale of software for the analysis of positron lifetime spectra
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Period: 01/01/2007 → …
Number of participants: 3
PALSfit
Acronym: PALSfit
Project participant:
Eldrup, Morten Mostgaard (Intern)
Kirkegaard, Peter (Intern)
Olsen, Jens V. (Intern)
Project

Resistance of Ni-Cermet anode supports against reduction-oxidation cycling: a step towards better durability of solid oxide fuel cells
Solid oxide fuel cells (SOFC) are a promising energy technology suitable for clean and efficient direct conversion of hydrogen carrying fuels into electricity and heat. The main potential market areas of SOFC systems are within distributed energy generation (combined heat and power) from small Residential applications up to MW class, and Auxiliary Power Units (APU) for both land and marine transport. The SOFC technology is currently under intensive research and development with an expected market entry of products within 1-3 years. Research and development are directed towards reducing cell and system cost, and improving the performance and durability of the cells under operation. The current project tackles the durability issue with the focus on a practical problem related to the operation of most current SOFC cells or systems, the so-called RedOx stability (= stability after a cycle of re-oxidation and reduction of an operating cell). The state-of-the-art SOFC anode is made of a composite of nickel and yttria stabilised zirconia. The anode supported cell design is operating at temperatures of 700-800 degrees Celsius with reducing atmosphere on the anode side. Due to cost issues, many small scale SOFC systems are not expected to have an inert sweep gas supply. In the case of fuel interruption, an oxidation of the nickel at these temperatures either severely degrades or completely destroys most current cells. The destruction is induced by the macroscopic expansion of the anode support, which results in destruction of the support itself and by cracking of the supported electrolyte layer. The large volumetric expansion is mainly caused by the phase change from Ni to NiO, which is the so called redox instability. The aim of the project has been to better understand the mechanisms and processes related to redox instability and through modifications to the half cell to improve the RedOx stability of Ni-based SOFC. We have demonstrated a redox stable Ni-YSZ composite and are in the process of implementing a modified structure into technologically relevant half cells. We have followed a pre-defined track of development work aiming to find microstructures and/or compositions that
enable more stable structures under a variety of operation conditions. In simple terms the redox instability is a thermo mechanical problem: excessive stresses in the layered ceramic cell structure may cause cracking and loss of tightness of the cell, with the electrolyte being the critical component. In the anode supported SOFC, the origin of the stress exerted on the electrolyte is the dimensional expansion of the anode support on re-oxidation. Therefore, the main goal of the development work was to design and manufacture anode substrates with improved dimensional stability during redox cycling. The target level, based on literature, was set to a linear expansion of 0.1 % on re-oxidation. The current anode substrate could not reach this target even at the mildest conditions. As a result of the project, we have gained an improved understanding on the processes of importance during redox cycling. We designed and manufactured several modified anode support substrates and the best of these reach the stability target of 0.1 % maximum expansion after 3 redox cycles at 850 oC under certain conditions. These results were based on modifications in the composite microstructure and composition by ceramic processing, by changing the sizes and distributions of particles and pores in the composite. Dopants were added to the nickel phase to improve the creep resistance and suppress nickel grain growth during operation or redox cycling. Within the project it was difficult to fully prove the effectiveness of these dopants compared to simultaneously introduced changes in microstructure. The implementation of the best modified anode support structures in technological half cells was started within this project. While knowledge about an improved anode support structure were obtained, further work in ceramic processing, mainly related to understanding sintering and co-sintering, is still needed to implement these structures in technologically relevant cells.

Department of Energy Conversion and Storage

Ceramic Engineering & Science
Period: 01/05/2006 → 30/04/2008
Number of participants: 1
fuel cell, SOFC, Ni-YSZ, Ni cermet, redox stability, sintering, continuum mechanics, kinetics, creep
Acronym: Redox stable SOFC
Project ID: 23882
Number of related Ph.D. students: 1
Project participant:
Kaiser, Andreas (Intern)

Financing sources
Source: EU research programme (public)
Name of research programme: FP6-Mobility
Amount: 189,549.00 Euro
Year of approval: 2006

Relations
Publications:
Strength of Anode-Supported Solid Oxide Fuel Cells
Continuum mechanics simulations of NiO/Ni-YSZ composites during reduction and re-oxidation
Curvature and Strength of Ni-YSZ Solid Oxide Half-Cells After Redox Treatments
Redox stability of SOFC: Thermal analysis of Ni-YSZ composites
Dimensional behaviour of Ni-YSZ anode supports for SOFC under redox cycling conditions
Testing and improving the redox stability of Ni-based SOFC
Mechanical properties of NiO/Ni-YSZ composites depending on temperature, porosity and redox cycling
Dimensional behavior of Ni-YSZ composites during redox cycling
Electrical conductivity of Ni–YSZ composites: Variants and redox cycling

Documents:
Thesis-Mikko-Pihlatie-P740
CORDIS_result_49143_en

Project

Activities:

Ceràmica (Journal)
Period: 2018
Vincenzo Esposito (Editor)
Department of Energy Conversion and Storage

Related journal
It is generally agreed that due to the increasing amount of renewable energy in the electricity production different energy conversion and storage technologies are needed to ensure a 100% availability of electricity.

Considering biomass as renewable source, fuel derived from landfill appears as attractive option. Landfill gas consists of carbon dioxide, methane and impurities as for example sulfur containing compounds. Combustion engines are often used to convert landfill gas into electricity and heat with the disadvantages of low efficiencies. Furthermore, most landfill gases are unattractive for combustion engines due to their low heating values.

One option to utilize landfill gases with a low heating value and to increase the electrical efficiency is the solid oxide fuel cell (SOFC). With SOFCs it is possible to convert hydrogen or carbon containing fuels, as for example landfill gas, directly into electricity and the side product heat in a highly efficient way.

To convert the landfill gas directly into electricity and heat in an SOFC, a reforming agent is needed to prevent carbon formation. Beside steam, it is possible to use carbon dioxide as a reforming agent (dry reforming). The advantage is that landfill gas already contains a certain amount of the needed carbon dioxide.
In the present work a planar 16 cm² SOFC cell was operated with a real landfill gas from one of the largest Danish waste
dump sites and additional carbon dioxide reforming agent at 750 °C, both with gas cleaning through an active carbon filter
and without. The tests showed an electric efficiency up to 60%. It was found that the active carbon filter was necessary to
prevent poisoning and thereby to decrease the degradation rate.
Degree of recognition: International
Links:
Conference)

Related event

7th EUROPEAN FUEL CELL PIERO LUNGHI CONFERENCE
12/12/2017 → 15/12/2017
Naples, Italy
Activity: Talks and presentations › Conference presentations

Reversible Operation using Carbonaceous Gasses of a 30-cell Solid Oxide Cell Stack
Period: 12 Dec 2017 → 15 Dec 2017
Søren Højgaard Jensen (Guest lecturer)
Hendrik Langnickel (Guest lecturer)
Nils Hintzen (Other)
Ming Chen (Guest lecturer)
Xifu Sun (Guest lecturer)
Anne Hauch (Guest lecturer)
Giacomo Butera (Guest lecturer)
Lasse Røngaard Clausen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Mixed Conductors
Department of Mechanical Engineering
Thermal Energy

Description
Recent theoretical studies show that reversible
electrochemical conversion of H2O and CO2 to CH4 inside novel
pressurized solid oxide cells (SOCs) combined with subsurface
storage of the produced gasses can facilitate seasonal electricity
storage with a round-trip efficiency 70-80% and a storage cost
below 3 ¢/kWh. Here we show test results from a 30-cell SOC
stack operated with carbonaceous gasses at 18.7 bar at 700 °C in
both electrolysis and fuel cell mode. The GC data from the
electrolysis test results show 18% methane in the dry outlet gas,
i.e. substantial methane formation inside the SOC stack. Further
we observed degradation rates comparable to that of ambient
pressure operation with H2/H2O gas mixtures.
Links:
Conference)

Related event

7th EUROPEAN FUEL CELL PIERO LUNGHI CONFERENCE
12/12/2017 → 15/12/2017
Naples, Italy
Activity: Talks and presentations › Conference presentations

Towards solid oxide electrolysis plants in 2020
Period: 28 Nov 2017
Ming Chen (Other)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Poster presentation
Degree of recognition: National

Related event
DEN DANSKE BRINT- OG BRÆNDELESCHELLEDA 2017
28/11/2017 → 28/11/2017
Odense, Denmark
Activity: Talks and presentations › Conference presentations

Wilson K. S. Chiu
Start date: 14 Nov 2017
Jacob R. Bowen (Host)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Synchrotron-based Hard X-Ray Microscopy: A Tool for 3-D Spectroscopic Imaging at the Nanoscale
Degree of recognition: International
Activity: Hosting a guest lecturer

Gerardina Carbone
Start date: 13 Nov 2017
Jacob R. Bowen (Host)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Brilliant opportunities with X-ray Nanobeams
Degree of recognition: International
Documents:
DTU_DCcarbone_Nov17
Activity: Hosting a guest lecturer

Perspectives in alkaline water electrolysis using membranes
Period: 3 Nov 2017
Mikkel Rykær Kraglund (Speaker)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: National
Documents:
DEF_PorouZ_JOEL_LTalk-projects

Related event
DEF Annual Meeting 2017
02/11/2017 → 03/11/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations
Keramiske membraner til ilblæst forgasning  
Period: 1 Nov 2017  
Astri Bjørnetun Haugen (Invited speaker)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science

Description
Arranger: IDA Mechanical  
Degree of recognition: National  
Links:  

Related event
UDVIKLING AF FREMTIDIGE METODER TIL PRODUKTION AF BIOBRÆNDSTOFFER OG GRØN ENERGI  
01/11/2017 → …  
Aarhus, Denmark  
Activity: Talks and presentations › Conference presentations

Advanced Concepts in Photovoltaics  
Period: 10 Oct 2017 → 13 Oct 2017  
Peter Behrensdorff Poulsen (Organizer)  
Gisele Alves dos Reis Benatto (Organizer)  
Jørgen Schou (Organizer)  
Department of Photonics Engineering  
Optical Microsensors and Micromaterials  
Organic Energy Materials

Description
Top Danish Researchers within photovoltaics was lecturing in this 4 day summer school along with Professor Peter Würfel, who is one of the international leading researchers within photovoltaics and author of the book Physics of Solar Cells: From Basic Principles to Advanced Concepts. The summer school was tailored towards PhD students within photovoltaics, but other interested in the program could join.  
Degree of recognition: International

Related event
Advanced Concepts in Photovoltaics: A Summer School in Photovoltaics  
10/10/2017 → 13/10/2017  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Progress in Photovoltaic Research in Denmark 2017  
Period: 9 Oct 2017  
Peter Behrensdorff Poulsen (Organizer)  
Gisele Alves dos Reis Benatto (Organizer)  
Department of Photonics Engineering  
Optical Microsensors and Micromaterials  
Organic Energy Materials

Description
For the conference we had assembled all the top researchers in Denmark within Photovoltaics to tell about their latest results. Furthermore, some of the highly innovative companies within photovoltaics in Denmark did elaborate on their newest achievements.  
Degree of recognition: International

Related event
Progress in Photovoltaic Research in Denmark 2017: Conference i Photovoltaics
09/10/2017 → …
Roskilde, Denmark
Activity: Attending an event › Participating in or organising a conference

12th International SDEWES Conference
Period: 6 Oct 2017
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage

Description
Held a presentation on: Integration of district cooling in smart energy systems: the case of Singapore
Degree of recognition: International

Related event
12th SDEWES Conference
04/10/2017 → 08/10/2017
Dubrovnik, Croatia
Activity: Talks and presentations › Conference presentations

Advanced fabrication of porous ceramic multilayers for membrane applications
Period: 2 Oct 2017
Andreas Kaiser (Keynote speaker)
Wenjing (Angela) Zhang (Invited speaker)
Manuel Pinelo (Invited speaker)
Michela Della Negra (Other)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Proton conductors
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Degree of recognition: International
Documents:
Icm 2017 - abstract - Andreas Kaiser

Related organisation
Advanced fabrication of porous ceramic multilayers for membrane applications
Kaiser, A. (Keynote speaker), Zhang, W. (. (Invited speaker), Pinelo, M. (Invited speaker), Della Negra, M. (Other)
2 Oct 2017
Activity: Talks and presentations › Conference presentations

In situ TEM study of the coarsening of carbon black supported Pt nanoparticles in hydrogen
Period: 1 Oct 2017 → 5 Oct 2017
Søren Bredmose Simonsen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
The control of sizes and shapes of nanostructures is of tremendous importance for the catalytic activity in electrochemistry and in catalysis more generally. However, due to relatively large surface free energies, nanostructures often sinter to form coarser and more stable structures that may not have the intended physicochemical properties.

Pt is known to be a very active catalyst in several chemical reactions and for example as carbon supported nanoparticles in fuel cells.

The presentation focusses on coarsening mechanisms of Pt nanoparticles supported on carbon black during exposure to
hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H2/Ar while ramping up the temperature to ca. 900 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in the pure hydrogen environment are stable during constant temperature ramping by 10°C/min up to ca. 800 °C. The coarsening above this temperature is fully dominated by the particle migration and coalescence mechanism. This is contrary to supported Pt nanoparticles in oxygen, where the coarsening is fully dominated by Ostwald ripening. For agglomerated Pt nanoparticles, coalescence events were observed already at ca. 200 °C. The temperature-dependency of particle sizes and the observed migration distances are consistent with simple early models for the migration and coalescence.

Degree of recognition: International

Related event

232nd ECS meeting
01/10/2017 → 05/10/2017
National Harbor, Washington, DC, United States
Activity: Talks and presentations › Conference presentations

NOMAD Summer
Period: 25 Sep 2017 → 29 Sep 2017
Simon Loftager (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

Related event

NOMAD Summer: A hands-on course on tools for novel-materials discovery
25/09/2017 → 29/09/2017
Berlin, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Fuel Cells (Journal)
Period: Aug 2017
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Links:

Related journal

Fuel Cells
1615-6846
Central database
Activity: Communication › Journal editor

SOFC/battery powered electrical vehicle
Period: Aug 2017 → Dec 2017
Anke Hagen (External examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
European Master in Renewable Energy
Activity: Examinations and supervision › Supervisor activities
Anode Catalyst Layer Contributing to the Overall Impedance of Polymer Electrolyte Membrane Electrolysis Cells during Water Electrolysis - A Hypothesis
Period: 30 Aug 2017
Katrine Elsøe (Guest lecturer)
Department of Energy Conversion and Storage

Related event
68th Annual Meeting of the International Society of Electrochemistry: Electrochemistry without Borders
27/08/2017 → 01/09/2017
Providence, United States
Activity: Talks and presentations › Conference presentations

The 15th International Conference on Advanced Materials IUMRS-ICAM
Period: 27 Aug 2017 → 1 Sep 2017
Ngo Van Nong (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
The 15th International Conference on Advanced Materials IUMRS-ICAM
27/08/2017 → …
Kyoto, Japan
Activity: Attending an event › Participating in or organising a conference

Blockchain Summer School 2017
Period: 14 Aug 2017 → 18 Aug 2017
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Description
Successfully participated in the summer school
Degree of recognition: International

Related event
Blockchain Summer School 2017
14/08/2017 → 18/08/2017
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Progress of SOFC/SOEC Development at DTU Energy: From Materials to Systems
Period: Jul 2017
Anke Hagen (Guest lecturer)
Peter Vang Hendriksen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry
Mixed Conductors

Related event
15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV)
23/07/2017 → 28/07/2017
Hollywood, United States
Activity: Talks and presentations › Conference presentations
**Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode**
Period: 23 Jul 2017 → 28 Jul 2017
Ming Chen (Other)
Department of Energy Conversion and Storage
Mixed Conductors

**Description**
Poster presentation.
Degree of recognition: International

**Related event**
15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV)
23/07/2017 → 28/07/2017
Hollywood, United States
Activity: Talks and presentations › Conference presentations

**Materials Optimization Using Advanced Computational Methods**
Period: 17 Jul 2017
Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

**Related event**
16/07/2017 → 21/12/2017
Easton, United States
Activity: Talks and presentations › Conference presentations

**Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017**
Period: 16 Jul 2017 → 30 Jul 2017
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage

**Description**
Successfully participated in the summer school.
Degree of recognition: International

**Related event**
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
16/07/2017 → 30/07/2017
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Advanced manufacturing of porous ceramic structures for use in energy applications**
Period: 10 Jul 2017
Andreas Kaiser (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Degree of recognition: International
Documents:
ecers2017-abstract-Andreas Kaiser
Links:
Related event

ECerS 2017 - 15th Conference & Exhibition of the European Ceramic Society: Advanced manufacturing of porous ceramic structures for use in energy applications
09/07/2017 → 13/07/2017
Budapest, Hungary
Activity: Talks and presentations › Conference presentations

30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Period: 5 Jul 2017
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Description
Gave a presentation on: "A multi-objective energy planning including system exergy efficiency and socio-economic costs"
Degree of recognition: International

Related event

30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
02/07/2017 → 06/07/2017
San Diego, United States
Activity: Talks and presentations › Conference presentations

3D Microstructural Evolution of a Solid Oxide Cell during a Redox Cycle by High Resolution Ptychographic Tomography
Period: 28 Jun 2017
Salvatore De Angelis (Guest lecturer)
Department of Energy Conversion and Storage
Description
3rd International Conference on Tomography of Materials and Structures
Degree of recognition: International
Links:

Related event

3rd International Conference on Tomography of 3D Materials and Structures
26/06/2017 → 30/06/2017
Lund, Sweden
Activity: Talks and presentations › Conference presentations

Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% -efficiency
Period: 26 Jun 2017 → 30 Jun 2017
Jørgen Schou (Guest lecturer)
Andrea Carlo Cazzaniga (Other)
Stela Canulescu (Other)
Andrea Crovetto (Other)
Rebecca Bolt Ettlinger (Other)
Nini Pryds (Guest lecturer)
Ole Hansen (Other)
Chang Yan (Other)
Kaiwen Sun (Other)
Xiaojing Hao (Other)
Department of Photonics Engineering
Optical Microsensors and Micromaterials
Multiphase oxygen electrodes for solid oxide electrolysis cells

Period: 22 Jun 2017
Dordije Tripkovic (Speaker)
Peter Vang Hendriksen (Other)
Mogens Bjerg Mogensen (Other)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Solid oxide electrolysis has the potential to become the most efficient way to convert electrical into chemical energy. Solid oxide electrolysis cells (SOEC) are thus an attractive solution for converting the occasional surplus amount of electricity produced by renewable energy sources to hydrogen or syngas. This promising technology requires further maturation to become economically competitive. Among other problems, the sluggish reaction at the oxygen electrode limits maximum fuel production rate, which directly affects overall process efficiency. Recent studies published by several groups highlight the importance of dissimilar interfaces and surface chemistry in promoting oxygen electrode reaction rate, opening a new route to enhance the electrode performance. Particularly, perovskite (113)/Ruddlesden-Popper (214) interface has been reported as highly beneficial for strontium doped lanthanum cobaltite (LSC) electrodes.[1–3]

The aim of this study is to investigate the potential of 113/214 interface to improve cobalt-free electrodes such as strontium doped lanthanum ferrite (LSF). The performance of LSF113/LSF214 couples is assessed by electrical conductivity relaxation (ECR) of geometrically well-defined electrodes, as well as by electrochemical impedance spectroscopy (EIS) of thin film electrodes prepared by PLD. The surface of the model electrodes is deliberately modified in a controlled manner by addition of secondary phases and examined by SEM and surface-sensitive characterization techniques.

Degree of recognition: International

Documents:
SSI21 abstract DJTRI

Links:
http://www.chimica.unipd.it/ssi21/ (The official conference website)

Related event
21st International Conference on Solid State Ionics
18/06/2017 → 23/06/2017
Padova, Italy
Activity: Talks and presentations › Conference presentations

The 40th International IAEE Conference
Period: 21 Jun 2017
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage

Description
Gave a presentation on: Potential of waste heat and waste cold energy recovery in Singapore for district cooling applications
Degree of recognition: International

Related event
40th Annual IAEE International Conference
18/06/2017 → 21/06/2017
Singapore, Singapore
Activity: Talks and presentations › Conference presentations

21st International Conference on Solid State Ionics
Period: 18 Jun 2017 → 23 Jun 2017
Vincenzo Esposito (Organizer)

Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Low-dimensional ionic and mixed ionic/electronic conductor nanostructures
Links:
http://www.chimica.unipd.it/ssi21/Symposium_II_1.html

Related event
21st International Conference on Solid State Ionics
18/06/2017 → 23/06/2017
Padova, Italy
Activity: Attending an event › Participating in or organising a conference

Demonstration of Impedance Spectroscopy as a Method to Evaluate Losses of Polymer Electrolyte Membrane Electrolysis Cells during Water Electrolysis
Period: 14 Jun 2017
Katrine Elsøe (Guest lecturer)

Department of Energy Conversion and Storage

Related event
International Conference on Electrolysis
12/06/2017 → 15/06/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Solid Oxide Electrolysis for Grid Balancing: Recent Achievements and Future Challenges
Period: 13 Jun 2017 → 15 Jun 2017
Ming Chen (Speaker)

Department of Energy Conversion and Storage
Mixed Conductors

Description
Solid oxide electrolysis is a promising technology for energy storage and synthetic fuel production and it has a unique potential for grid regulation in the Danish power system. In this presentation results from the recent ForskEL projects coordinated by DTU Energy on developing the SOEC technology were presented.
Degree of recognition: International

Related event
Alkaline membrane electrolysis with PEM-level electrochemical performance
Period: 12 Jun 2017
Mikkel Rykær Kraglund (Guest lecturer)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: International
Documents:
ICE2017_KraglundMR_Alkaline membrane electrolysis with PEM-level electrochemical performance

Related event

Tutorial on high-throughput computations
Period: 29 May 2017 → 31 May 2017
Simon Loftager (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
MARVEL/MaX/Psi-k tutorial on high-throughput computations: General methods and applications using AiiDA
Degree of recognition: International

Related event

Tutorial on high-throughput computations: General methods and applications using AiiDA
29/05/2017 → 31/05/2017
Lausanne, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

EMRS Spring meeting 2017
Period: 23 May 2017
Jørgen Schou (Participant)
Andrea Carlo Cazzaniga (Participant)
Stela Canulescu (Organizer)
Rebecca Bolt Ettlinger (Participant)
Nini Pryds (Participant)
Ole Hansen (Organizer)
Andrea Crovetto (Organizer)
Chang Yan (Participant)
Kaiwen Sun (Participant)
Xiaojing Hao (Participant)
Department of Photonics Engineering
Photovoltaic Materials and Systems
Optical Microsensors and Micromaterials
Department of Energy Conversion and Storage
Electrofunctional materials
Experimental Surface and Nanomaterials Physics
Department of Micro- and Nanotechnology
Silicon Microtechnology
Department of Physics

Description
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency
Degree of recognition: International
Documents:
Abstract Earth-abundant CZTS

Related event
EMRS Spring meeting 2017
22/05/2017 → 26/05/2017
Strasbourg, France
Activity: Attending an event › Participating in or organising a conference

Topics in Mining, Metallurgy and Materials Engineering (Journal)
Period: 18 May 2017
Vincenzo Esposito (Editor)
Ceramic Engineering & Science
Department of Energy Conversion and Storage

Description
Topics in Mining, Metallurgy and Materials Engineering

Related journal
Topics in Mining, Metallurgy and Materials Engineering
2364-3293
Local database
Activity: Research › Journal editor

Materials Research Society Spring Meeting 2017
Period: 17 Apr 2017 → 21 Apr 2017
Jørgen Schou (Organizer)
Andrea Carlo Cazzaniga (Participant)
Andrea Crovetto (Participant)
Rebecca Bolt Ettlinger (Participant)
Sara Lena Josefin Engberg (Participant)
Stela Canulescu (Participant)
Nini Pryds (Participant)
Ole Hansen (Participant)
Chang Yan (Participant)
Kaiwen Sun (Participant)
Xiaojing Hao (Participant)
Department of Photonics Engineering
Photovoltaic Materials and Systems
Department of Physics
Experimental Surface and Nanomaterials Physics
Optical Microsensors and Micromaterials
Description
Pulsed laser deposition (PLD) of a CZTS-absorber for thin solar cells with up to 5.2 % efficiency
Degree of recognition: International
Documents:
MRS 2017_poster_JS_2

Related event
Materials Research Society Spring Meeting 2017
17/04/2017 → 21/04/2017
Phoenix, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Phosphoric Acid Anion Migration through Polybenzimidazole Membrane
Period: 9 Apr 2017
Hans Becker (Speaker)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: International

Related event
CARISMA Conference 2017
09/04/2017 → 12/07/2017
Newcastle, United Kingdom
Activity: Talks and presentations › Conference presentations

Udfordringer ved VE-gas anvendt i brændselsceller
Period: 22 Mar 2017
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Invited talk

Related event
IDA KEMI
22/03/2017 → 22/03/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Workshop for electromechanical and dielectric materials and devices
Period: 9 Mar 2017
Astri Bjernetun Haugen (Organizer)
Hugh Simons (Organizer)
Department of Energy Conversion and Storage
DFT Studies of the ORR Activity of Carbon Encapsulated Fe3C
Period: 1 Mar 2017
Heine Anton Hansen (Other)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International
Related event
European Fuel Cell Car Workshop
01/03/2017 → 03/03/2017
Orleans, France
Activity: Talks and presentations › Conference presentations

MODELING OF LI-ION BATTERY PACKS AS BASIS FOR DESIGN OF BATTERY THERMAL MANAGEMENT SYSTEMS
Period: 6 Feb 2017
Kurt Engelbrecht (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
External opponent on PhD thesis
Degree of recognition: National
Activity: Examinations and supervision › External examination

41st International Conference and Expo on Advanced Ceramics and Composites
Period: 22 Jan 2017 → 27 Jan 2017
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
14th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology
Links:
http://ceramics.org/icacc17-s3
Related event
41st International Conference and Expo on Advanced Ceramics and Composites
22/01/2017 → 27/01/2017
Florida, United States
Activity: Attending an event › Participating in or organising a conference
Ceramic processing of tubular, multilayered oxygen transport membranes (Invited)
Period: 22 Jan 2017 → 27 Jan 2017
Astri Bjørnetun Haugen (Invited speaker)

Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Pure oxygen gas supplied by ceramic oxygen transport membranes (OTMs) can facilitate reduced CO2 emissions through more efficient gasification or combustion processes and easier CO2 capture and storage. For maximum oxygen flux and 100% selectivity, the active OTM layer should be thin and dense, and have a large and catalytically activated surface area. These requirements call for an asymmetric OTM design with a thin, dense OTM layer (~15 μm) sandwiched between two porous catalyst layers (~15 μm) and mechanically supported on a porous ceramic substrate (~1 mm).

This talk pertains to our work at the Technical University of Denmark (DTU) related to processing such multilayered ceramic components with a tubular geometry, focusing on scalable process technologies. This includes thermoplastic extrusion to shape the porous, tubular support, deposition of thin dense and porous layers by dip coating, co-sintering of these layers, and infiltration of electrocatalysts. Material and processing considerations for two different combinations of materials in the multilayered components will be discussed, and performance of these components under laboratory testing and integrated in pilot-scale biomass gasifiers will be presented.

Degree of recognition: International
Documents:
Abstract_ICACC217

Related event

41st International Conference and Expo on Advanced Ceramics and Composites
Period: 22/01/2017 → 27/01/2017
Florida, United States
Activity: Talks and presentations › Conference presentations

Thermo-mechanical properties of Metal-supported Solid Oxide Fuel Cells components
Period: 22 Jan 2017 → 27 Jan 2017
Francesca Teocoli (Speaker)

Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
41st Int'l Conf & Expo on Advanced Ceramics & Composites (ICACC 2017)
Degree of recognition: International

Related external organisation
The American Ceramic Society
United States
Activity: Talks and presentations › Conference presentations

Period: 2016
David Aili (Speaker)

Department of Energy Conversion and Storage
Proton conductors
Description
Ternary alkaline polybenzimidazole-based electrolytes

Related event
13/06/2016 → 16/06/2016
Zaragoza, Spain
Activity: Talks and presentations › Conference presentations

ChemSusChem (Journal)
Period: 2016
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal
ChemSusChem
1864-5631
Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts

Direct use of biogas in SOFC
Period: 2016
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Kandidatspeciale
Coordinated by Anke Hagen
Activity: Other

ELSEVIER (Publisher)
Period: 2016
Vincenzo Esposito (Editor)
Ceramic Engineering & Science
Department of Energy Conversion and Storage

Description
Metal Oxide-Based Thin Film Structures
Degree of recognition: International
Links:
https://www.elsevier.com/books/metal-oxide-based-thin-film-structures/pryds/978-0-12-810418-7

Related Publisher
ELSEVIER
Local database
Activity: Research › Series editor

Journal of Industrial and Engineering Chemistry (Journal)
Period: 2016
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related journal**

**Journal of Industrial and Engineering Chemistry**
1226-086X
Central database
Activity: Research › Peer review of manuscripts

**Journal of Power Sources (Journal)**
Period: 2016
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related journal**

**Journal of Power Sources**
0378-7753
Central database
Activity: Research › Peer review of manuscripts

**Kopernikus PsX (External organisation)**
Period: 2016 → 2026
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
International Advisory Board member

**Related external organisation**

**Kopernikus PsX**
Germany
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**PhD Thesis Kristian B. Knudsen: Censor**
Period: 2016
Anke Hagen (Internal examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Censor
Activity: Examinations and supervision › Internal examination

**Polish Science Foundation (External organisation)**
Period: 2016
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Evaluation of proposals

Related external organisation

Polish Science Foundation
Poland
Activity: Membership › Membership in review committee

Solid State Protonic Conductors 18
Period: 2016
David Aili (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
Acid-base chemistry and proton conductivity of solid acids and their mixtures with N-heterocycles

Related event

Solid State Protonic Conductors 18
18/09/2016 → …
Oslo, Norway
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Ternary polybenzimidazole-based alkaline electrolytes
Period: 2016
David Aili (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Related event

Workshop on Ion Exchange Membranes for Energy Applications
27/06/2016 → …
Bad Zwischenahn, Germany
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs (External organisation)
Period: 2016
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Evaluation of proposals

Related external organisation

Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs
Austria
Activity: Membership › Membership in review committee

Integrated computational and experimental design of next-generation battery materials
Period: 9 Dec 2016
Tejs Vegge (Invited speaker)
As a part of my stay at NTU in collaboration with Energy Research Institute at NTU, I was developing models for assessment of district cooling (DC) potential in Singapore. The work consisted of mapping the energy resources and potential DC demand, analyzing demand patterns, conducting pre-feasibility studies and evaluating the possibility of developing DC system on a large scale.

In the second part of the project integration of DC with the energy system was assessed. Synergies between different energy sectors were detected and the potential for utilizing them was evaluated. It was found that the DC should contribute to the overall goal of reducing GHG emissions, established by the government of Singapore, as well as to increase energy security of the country.

Results will be presented at IAEE2017 conference in Singapore in June 2017.

Links:
http://erian.ntu.edu.sg/Pages/Home.aspx
7th European Kesterite Workshop
Period: 17 Nov 2016 → 18 Nov 2016
Christian Rein (Participant)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
CZTS synthesis using deep eutectic solvents.

Related event
7th European Kesterite Workshop
16/11/2016 → 18/11/2016
Leuven, Belgium
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Solid-State Li-S Batteries based on Borohydride Solid Electrolyte
Period: 17 Nov 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Materials Research Society of Korea: MRS-K 2016 Fall meeting
16/11/2016 → 18/11/2016
Gyeongju, Korea, Republic of
Activity: Talks and presentations › Conference presentations

Solid-State Li-S Batteries based on Borohydride Solid Electrolyte
Period: 16 Nov 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
9th International Workshop on EEWS
15/11/2016 → 16/11/2016
Daejeon, Korea, Republic of
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Computational methods for accelerated DFT-based design of energy materials
Period: 8 Nov 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
TUM Energy Colloquium
08/11/2016 → 08/11/2016
München, Germany
Activity: Talks and presentations › Conference presentations
High Performance Thermoelectric Materials and Modules for Harvesting Waste Heat
Period: 8 Nov 2016 → 12 Nov 2016
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
The 8th International Workshop on ADVANCED MATERIALS SCIENCE AND NANOTECHNOLOGY
08/11/2016 → 12/11/2016
Activity: Talks and presentations › Conference presentations

August Wilhelm Scheer
Start date: 6 Nov 2016 → 11 Nov 2016
Tejs Vegge (Host)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Activity: Hosting a guest lecturer

Processing parameters and raw material influence on the microstructure and performance of SiC membranes for water filtration
Period: 2 Nov 2016 → 3 Nov 2016
Michela Della Negra (Lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event
16th Aachener membrane Kolloquium
02/11/2016 → 03/11/2016
Aachen, Germany
Activity: Talks and presentations › Conference presentations

Materials Science & Technology 2016 (MS&T16) conference
Ming Chen (Invited speaker)
Department of Energy Conversion and Storage
Mixed Conductors
Links:
http://www.matscitech.org/technical-program/fundamentals-and-characterization/

Related event
Materials Science & Technology 2016 (MS&T16) conference: Phase Stability, Diffusion Kinetics, and Their Applications (PSDK-XI) Symposium
23/10/2016 → 27/10/2016
Salt Lake City, United States
Activity: Talks and presentations › Conference presentations

From CO2 to Sustainable Fuels and Chemicals
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Oral and poster presentations

EU-US Frontiers of Engineering Symposium
17/10/2016 → 19/12/2016
Helsinki, Finland
Activity: Talks and presentations › Conference presentations

69th Annual Gaseous Electronics Conference
Period: 10 Oct 2016
Ming Chen (Invited speaker)
Department of Energy Conversion and Storage
Mixed Conductors

Related event
69th Annual Gaseous Electronics Conference: Session BM1: Electrification of the chemical Industry
10/10/2016 → 10/10/2016
Bochum, Germany
Activity: Talks and presentations › Conference presentations

Computational design of nanoalloys using DFT calculations, genetic algorithms and machine learning
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
8th International Conference on Multiscale Materials Modeling
09/10/2016 → 14/10/2016
Dijon, France
Activity: Talks and presentations › Conference presentations

PRIME 2016/230th ECS Meeting
Period: 6 Oct 2016
Yang Hu (Speaker)
Department of Energy Conversion and Storage
Proton conductors

Description
oral presentation: Probing the active site structures of iron-based ORR catalysts

2016PRIME-230th Meeting of The Electrochemical Society (ECS)

Related event
PRIME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations

Denmark-China Bilateral Workshop on Energy Conversion and Storage
Ming Chen (Organizer)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Denmark-China Bilateral Workshop on Energy Conversion and Storage
Links:
http://www.energy.dtu.dk/english/News/Nyhed?id=31bf51e9-f572-4e45-8a11-c3d277750ed5

Related event
Denmark-China Bilateral Workshop on Energy Conversion and Storage
03/10/2016 → 04/10/2016
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Electrochemical Characterization of PEMECs Operating at Various Current Densities
Period: 2 Oct 2016
Katrine Elsøe (Guest lecturer)
Department of Energy Conversion and Storage

Related event
PRiME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations

EXPERIMENTAL PROOF OF CONCEPT OF A PIEZOELECTRIC-SHAPE MEMORY ENERGY HARVESTER
Period: 2 Oct 2016 → 2 Apr 2017
Kurt Engelbrecht (Supervisor)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
The aim of this work is the experimental proof of concept of an energy harvester using shape memory effect and piezoelectricity to transform input thermal power in output electricity. The practice of recovering wasted or unused energy from the environment and making it available in form of electrical charge – i.e. energy harvesting – is attracting increasing attention since it can be employed for feeding small wireless autonomous devices as a valid alternative to batteries or grid connection. As a matter of facts, traditional solutions imply continuous maintenance (e.g. batteries need to be substituted periodically) or non-economical arrangements (e.g. connecting to the grid very small devices in remote locations is not only complicated but also anti economical). Energy harvesting then addresses the problem of feeding low-power electronics and autonomous wireless sensors (requiring few mW of electricity).

Since this field of research is pretty new, not much literature is available on the topic but on the other side lot of work and improvement can be done; moreover, there is not a recognized best way of doing things, then experimental activity needs to be performed to explore possible solutions.

In this work the problem of energy harvesting is addressed to considering thermal energy as available source input, to be transformed in electrical power; this is the starting point: all that comes after is the result of studies performed within this thesis. The first step is deciding which mechanism to be employed: the choice is to use shape memory effect of Ni-Ti for converting thermal power into mechanical one and then a piezoelectric actuator that receives mechanical power as an input and converts it into electricity. The reason for that is double: on one side, a research group already provided a similar device that could be used as reference and improved; on the other, Ni-Ti is the object of ongoing research due to its incredible properties and then it is due to contribute in experiments by providing another type of application for this material.

The second step is then gathering information on shape memory alloys and piezoelectric components from literature and manufacturers and designing an experimental session to provide the other pieces of information needed for the realization of this device.

Starting from shape memory effect, it is a property exhibited by certain materials that can restore the original shape of a plastically deformed sample by simply heating it as a consequence of a crystalline phase change – called martensitic transformation. In particular, at low temperature, below the transformation starting one, the material is in martensitic phase, which is soft and can be deformed quite easily. Then, when the specimen is heated up above a transition starting temperature, it recovers its original pre-deformation shape and converts the material to its high strength – austenitic – condition. The process is reversible, meaning that the same transformation occurs while cooling, even though some
hysteresis can be detected and temperature range is slightly different. If the specimen is in a constrained configuration, i.e. it cannot recover its initial shape upon heating due to zero displacement constrains, force starts growing inside it; then, it goes down while cooling. These properties are known from literature. The problem is that it is not clear how force depends on temperature and which are relevant variables affecting performance: for this reason an experimental characterization is performed. First of all, a shape memory alloy is selected, in particular Ni-Ti due to its above the average properties, even though there are also other different classes of materials showing this effect. Then a bundle of wires of Ni-Ti is tested, considering that output force depends on cold wires temperature, hot wires temperature and pre-stress, meaning force applied to the specimen at cold state, before it is heated up and actuation, i.e. force, produced. Characterization is made for a limited but still meaningful temperature values and for a wide range of pre-stress. Results show that the best operating temperatures are 5 °C as cold temperature and 55 °C as hot one, being temperature difference fixed at 50 °C. Force difference between hot and cold states increases with pre-stress almost linearly; for this reason, a pre-stress of 1000 N is selected as the one to be employed in the device during operations. Actuation provided with these parameters is expected to be 600 N.

Moving to piezoelectricity, it is the property of producing electrical charge when submitted to a certain pressure (direct piezoelectric effect), manifested by a specific class of materials. Nowadays there are many devices employing the opposite effect – inverse piezoelectricity: they receive voltage as input and produce displacement as an output; knowing the relation between displacement and voltage it is possible to provide precise control. Among these materials, the most common one is Lead Zirconate Titanate due to its marked piezoelectric effect. Working principle is as follows: when subjected to a force, there is a shifting of electrons in the crystal structure of this material, resulting in a charge; this process is reversible in a certain range of temperature, force and electric field, meaning that if force is removed the electrons go back to initial configuration and charge goes back to zero. While inverse piezoelectric effect is well known, direct one is pretty unstudied due to limited number of practical applications: for this reason a sample of Lead Zirconate Titanate needs to be tested and characterized. The goal is to find how voltage depends on force (current is expected to be very small, while voltage relevant, for this reason it is selected as variable for evaluating the performance). In the experimental session the piezoelectric actuator is then compressed at increasingly high force and voltage is measured; moreover, the effect of compression speed is investigated since it could be a relevant variable considering that a transformation in the crystal occurs. Results show that absolute value of voltage increases almost linearly with force: when compressed the actuator produces positive voltage; then if it is shortened at maximum force and gradually released to zero stress, a negative voltage builds up: for this reason it is convenient to speak about potential difference per cycle. At 600 N, which is the force provided by Ni-Ti, potential difference is expected to be between 25 V and 35 V in relation to compression speed, which slightly affects output.

Once the properties of the two main components are clear, a device employing them is designed and built. A globally zero displacement assembly is chosen: Ni-Ti wires are clamped together with the piezoelectric actuator and then subjected to temperature fluctuation, so that they produce a force that alternatively compresses and releases the piezo, finally generating in this way an electrical charge. Water is selected as heat transfer fluid and 13 wires of 5 mm length and 0.8 mm diameter of active part are disposed circularly, perpendicularly to the flow in an optimized configuration in terms of heat transfer, held in place by plastic plates and put inside a cylindrical case. A shaft then puts the active part in connection with piezoelectric actuator, well separating it from the flow since it is not waterproof. While designing this assembly, great care is reserved to heat transfer problem and to a detailed study of how stress/strain state should evolve during operation. As regards heat transfer, both manual computation and numerical simulations are performed in order to find a configuration where water and wires exchange heat properly, i.e. effectively, homogeneously and fast. As a matter of facts, non-homogeneous heat transfer with the wires would result in uneven shape memory effect and then in differential displacement; moreover, being the slowest phenomenon, heat transfer affects operating frequency of the whole device: for this reason it needs to be analyzed carefully. Stress/strain problem is also studied in details, cross-referencing data from both literature and experiments: it is fundamental to design the length and number of wires compatibly with stress and displacement required by piezo, which in turn depends on shape memory effect at a given temperature. In other words, it is mandatory to run a trial and error process, where there are different involved variables that need to be compatible one with the others in order to have the device working. These studies show that aforementioned configuration of 13 wires of 5 mm length and 0.8 mm diameter is a solution to this problem; even though it is not the optimized one, it should work properly for a proof of concept.

Getting back to design, there are then auxiliary elements, in particular a hydraulic circuit composed of two identical lines, one for the hot and one for the cold side, alternatively switched by means of three way valves. Water baths provide temperature control and water flow. Their goal is exchanging heat with active part of the device, providing desired temperature change at a given frequency. The other auxiliary element is the electrical circuit, aimed at collecting and measuring the charge produced by the piezo; the main components are a series of two resistors of known resistance coupled with a voltmeter for reading the voltage and a relay for switching the circuit on and off. In particular, since generated charge is very small, it is necessary first to build up a voltage across the piezo and then to discharge it across the measurement system within a certain frequency.

Finally, there is a control/data acquisition system based on LabVIEW aiming at measuring temperatures with thermocouples and recording it and at automatically switch electrical circuit with a small control current while recording voltage. Once all the parts are designed, they are built and assembled and tests are run on the apparatus. Experimental setup consists in the aforementioned components, clamped with a mechanical actuator and operating as follows. The mechanical actuator provides 1000 N of pre-stress while maintaining a zero displacement configuration; the assembly...
made of a cylinder containing Ni-Ti active component and a shaft for rigidly transmitting force to the piezo chip is blocked between the two plates of the mechanical actuator. Two hoses connect active chamber to hydraulic circuit while two wires connect piezo to electrical circuit. Data acquisition system completes the setup. As regards operation, several experiments are done to find best working point. Sequence of operations is as follows: pre-stress is provided while cold water is circulating, then circuit is closed to discharge voltage built up by the pre-stress and opened after that; these are preliminary actions. Then, three-way valves are switched so hot water flows and heats up the wires, which expand and actuate on the piezo, generating a voltage that can be measured after closing the circuit; the circuit is then re-opened, valves switched to cold water and then a negative voltage builds up across the piezo; electrical circuit is closed again and negative voltage measured, then it is re-opened. At this point, a new cycle begins. Data acquisition saves temperature to time and voltage to time.

These data are then elaborated employing a MATLAB script where total voltage, current, power and energy harvested per cycle are measured. Results are very positive: a potential difference of 30.73 V and a current of 2.82 mA are detected; power is 44.46 mW, while harvested energy per cycle is 0.33 mJ. An efficiency index which reports harvested energy per cycle to the mass of active part – Ni-Ti – is defined and computed: it is 2.04 mJ/g. These numbers not only prove the concept of energy harvesting, but also highlight a performance that is much better than previous devices and then can be considered as a good starting point for future developments.

In particular, an optimization process of existing device is suggested as it could improve the performance dramatically. In the following there is a list of suggestions on what could be done. First of all, an observation is mandatory: this thesis is a proof of concept, meaning that there are no requirements in terms of performance, dimensions and output of the device; when designing an energy harvester for a specific application, starting point should always be electrical requirements from the load and then design should follow up. The point is that completely different devices could be built according to the kind of application: the only element in common would be the working principle. Future developments for this specific design can be summarized as follows. First of all, from a Ni-Ti point of view it could be interesting to increase the number of wires for providing a higher actuation and a bigger pre-stress as operating condition, impossible now due to limited yield strength as failure tests show. Another improvement could be made in relation to hydraulic circuit and heat transfer: in this device operating frequency is fairly slow because the temperature of heat transfer fluid is the same as Ni-Ti desired one and valves are manual. It could be possible to design automatic valves and employ higher temperature difference so that desired temperature of Ni-Ti would be reached faster and at this point valves would switch automatically. As a result, system would operate with higher frequency and then also global harvested energy would be bigger, due to more cycles in the same time interval. Finally, a wider characterization of temperature influence on Ni-Ti displacement could lead to the definition of better working conditions.

Degree of recognition: International
Documents:
2017_04_Bazzan
Activity: Examinations and supervision › Supervisor activities

**Genetic Algorithms and DFT for Accelerated Design of Nanoalloys**

Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

**Related event**

**PRIME 2016/230th ECS Meeting**
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations

**PRIME 2016/230th ECS Meeting**
Period: 2 Oct 2016
Salvatore De Angelis (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Description**
Electrochemical society meeting. Oral presentation
Related event

PRiME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Attending an event › Participating in or organising a conference

In situ X-ray diffraction studies of electrode materials in working metal-ion batteries and other layered materials
Period: 20 Sep 2016
Rune E. Johnsen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Imaging and Structural Analysis

Description
Seminar talk at Physics Department, Technical University of Munich

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Error Identification in DFT for Sustainable Energy Technologies
Period: 15 Sep 2016
Rune Christensen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Seminar talk at Brown University

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

7th International Conference on Magnetic Refrigeration at Room Temperature (Thermag VII)
Period: 11 Sep 2016 → 14 Sep 2016
Christian Bahl (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

7th International Conference on Magnetic Refrigeration at Room Temperature (Thermag VII)
Turin, Italy
Activity: Talks and presentations › Conference presentations

Brown University
Period: 11 Sep 2016 → 18 Sep 2016
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Visit at Brown University: Catalyst Design Lab
11th Conference on Sustainable Development of Energy, Water and Environment Systems
Period: 4 Sep 2016 → 9 Sep 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Attended the conference and hold a presentation on "Improving the Performance of District Heating Systems by Utilization of Local Heat Boosters"
Degree of recognition: International
Links:
http://www.lisbon2016.sdewes.org/

Related event
11th Conference on Sustainable Development of Energy, Water and Environment Systems
04/09/2016 → 09/09/2016
Lisbon, Portugal
Activity: Talks and presentations › Conference presentations

Quasi-Elastic Neutron Scattering studies for Material Research
Period: 2 Sep 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
50 Years of Neutron Backscattering
02/09/2015 → 03/12/2016
Munich, Germany
Activity: Talks and presentations › Conference presentations

Dänemark ohne fossile Brennstoffe: Möglichkeiten für die Hochtemperaturbrennstoffzelle und Elektrolyse
Period: Aug 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Invited talk

Related event
Kopernikus P2X Kolloquium
24/10/2016 → 25/10/2016
Jülich, Germany
Activity: Talks and presentations › Conference presentations

SOFC/SOEC in Dänemark – Status und Herausforderungen in einer neuen Finanzierungslandschaft
Period: Aug 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
**Description**
Invited talk

**Related event**

**DACH 4 SOFC/SOEC Treffen**
17/10/2016 → 18/10/2016
Jülich, Germany
Activity: Talks and presentations  Conference presentations

**Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for all-solid-state Lithium Batteries**
Period: 30 Aug 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

**European Crystallographic Meeting 2016**
28/08/2016 → 01/09/2016
Basel, Switzerland
Activity: Talks and presentations  Conference presentations

**IN-SITU TRANSMISSION ELECTRON MICROSCOPY ON OPERATING ELECTROCHEMICAL CELLS**
Fabrizio Gualandris (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Description**
Partecipation at The European Microscopy Congress (EMC) 2016 with a talk. EMC is an international conference of the highest quality sitting alongside Europe's largest exhibition dedicated to microscopy. In addition to the conference and exhibition there will be great training opportunities, a programme of technical workshops, and a full social programme.
Degree of recognition: International
Documents:
Abstract
Links:
http://emc-proceedings.com/abstract/in-situ-transmission-electron-microscopy-on-operating-electrochemical-cells/
(Abstract)

**Related organisation**

**IN-SITU TRANSMISSION ELECTRON MICROSCOPY ON OPERATING ELECTROCHEMICAL CELLS**
Gualandris, F. (Speaker)
28 Aug 2016 → 2 Sep 2016
Activity: Talks and presentations  Conference presentations

**SOCs for various occasions**
Period: 24 Aug 2016
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

**Related event**

**International Congress on Ceramics (ICC6)**
21/08/2016 → 25/08/2016
Dresden, Germany
Activity: Talks and presentations  Conference presentations
67th Annual Meeting of the International Society of Electrochemistry in The Hague
Heine Anton Hansen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description

Related event
67th Annual Meeting of the International Society of Electrochemistry: Electrochemistry: from Sense to Sustainability
21/08/2016 → 26/08/2016
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

2016 CAMD Summer School on Electronic Structure Theory and Materials Design
Tejs Vegge (Organizer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Electrochemical Energy Conversion and Storage
c{o-organizer and speaker

Related event
2016 CAMD Summer School on Electronic Structure Theory and Materials Design
14/08/2016 → 19/08/2016
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Atomic Scale Modeling of Electrocatalytic Reactions
Period: 12 Aug 2016
Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
Seminar titled "Atomic Scale Modeling of Electrocatalytic Reactions" at the Scott Institute, Carnegie Mellon University, Pittsburgh.

Related event
Atomic Scale Modeling of Electrocatalytic Reactions
12/08/2016 → …
Pittsburgh, United States
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities
15th International Symposium on Metal-Hydrogen Systems
Period: 10 Aug 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Complex Hydrides as room-temperature solid electrolytes for rechargeable batteries
Oral Presentation

Related event
15th International Symposium on Metal-Hydrogen Systems
07/08/2016 → 12/08/2016
Interlaken, Switzerland
Activity: Talks and presentations › Conference presentations
Computational Design of Materials for Hydrogen Storage, Batteries and Electrocatalysis
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
15th International Symposium on Metal-Hydrogen Systems
07/08/2016 → 12/08/2016
Interlaken, Switzerland
Activity: Talks and presentations › Conference presentations
Summer school on Smart Energy Systems and Entrepreneurship
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities
Description
Participated in and gave a pitch on "Bioliq" start-up.
Participated in and presented a pitch at the Summer school on Smart Energy Systems and Entrepreneurship organized by EIT digital and Karlsruhe Institute of Technology, Karlsruhe, Germany

Related event
Summer school on Smart Energy Systems and Entrepreneurship
25/07/2016 → 05/08/2016
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations
Bayesian statistics to improve accuracy through identification and correction of systematic errors in DFT
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
CEA-TUM Summer School on the Future of a Common European Strategy
Period: 6 Jul 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Participated in a summer school and presented a poster during both poster and rapid fire sessions.

Participated and presented a poster at the CEA-TUM Summer School on the Future of a Common European Strategy at Abtei Frauenwörth, Bavaria, Germany

Related event
CEA-TUM Summer School on the Future of a Common European Strategy
05/07/2016 → 10/07/2016
Chiemsee, Germany
Activity: Talks and presentations › Conference presentations

Presentation of DTU Energy: by Professor Søren Linderoth
Period: 6 Jul 2016
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage
Activity: Other

12th European SOFC & SOE Forum 2016
Period: 5 Jul 2016 → 8 Jul 2016
Ming Chen (Speaker)
Department of Energy Conversion and Storage
Mixed Conductors

Related event
12th European SOFC & SOE Forum
05/07/2016 → 08/07/2016
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations

Workshop on Ion Exchange Membranes for Energy Applications
Andreas Kirkebæk (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
Comparative Study of the Effect of Various Cross Linkers upon Membrane Properties

Poster presentation
Documents:
EMEA2016 Poster - Andreas Kirkebæk

Related event
Workshop on Ion Exchange Membranes for Energy Applications
27/06/2016 → …
Bad Zwischenahn, Germany
Activity: Attending an event › Participating in or organising a conference

29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
Period: 21 Jun 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Gave a presentation on: "Benefits of Integrating Geographically Distributed District Heating Systems"

ECOS 29th International Conference
Documents:
Dominkovic_Benefits of Integrating Geographically Distributed District Heating Systems_presentation

Related event
29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
19/06/2016 → 23/08/2016
Portorož, Slovenia
Activity: Talks and presentations › Conference presentations

Computational Design of Materials for Electrochemical Energy Storage at DTU Energy
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage

Related event
1st Lancaster University-DTU Electrochemistry Workshop
21/06/2016 → 22/12/2016
Lancaster, United Kingdom
Activity: Talks and presentations › Conference presentations

Trends and frontiers in solid state energy conversion - materials and technologies
Period: 20 Jun 2016
Christian Bahl (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Energy conversion using solid state materials allows for simple and compact devices that can be used in energy applications. A range of materials exist which can be used for such solid state energy conversion. The best known ones are maybe the thermoelectric materials that can generate electricity from a temperature span or vice versa. The so-called caloric materials will change their temperature when exposed to an external field, which may be magnetic, electrical or mechanical. These can be used either for heat pumping, or for generating energy from waste heat. The available materials for solid state energy conversion technologies will be reviewed and the present state of the art of these technologies will be discussed.

Related event
29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
19/06/2016 → 23/08/2016
Portorož, Slovenia
Activity: Talks and presentations › Conference presentations
6th Baltic Electrochemistry Conference
Period: 17 Jun 2016
Marko Melander (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Participation and presentation at the 6th Baltic Electrochemistry Conference

Related event

6th Baltic Electrochemistry Conference
15/06/2016 → 17/06/2016
Helsinki, Finland
Activity: Talks and presentations › Conference presentations

2nd South East European Conference on Sustainable Development of Energy, Water and Environment Systems
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
I gave a presentation on: "Modelling transition towards sustainable transportation sector". I was coauthor of two additional papers that were presented during the conference.

Documents:
Dominkovic_Modelling transition towards sustainable transportation sector

Related event

2nd South East European Conference on Sustainable Development of Energy, Water and Environment Systems
15/06/2016 → 18/08/2016
Piran, Slovenia
Activity: Talks and presentations › Conference presentations

Nanoconfined LiBH4 in mesoporous silica scaffold as solid electrolyte for solid-state Lithium battery
Period: 14 Jun 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

EMN Meeting on mesoporous materials: EMN
13/06/2016 → 17/06/2016
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

Hydrogen2Storage & Transport in Denmark
Period: 8 Jun 2016
Ming Chen (Participant)
Department of Energy Conversion and Storage
Mixed Conductors
Related event

**Hydrogen Storage & Transport in Denmark**
08/06/2016 → 08/06/2016
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**GPAW 2016: Users and developers meeting**
Marko Melander (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
GPAW developers meeting

**Related event**

**GPAW 2016: Users and developers meeting**
06/06/2016 → 10/06/2016
Jyväskylä, Finland
Activity: Talks and presentations › Conference presentations

**Effect of fast mass diffusion regime on defective ceria mechano-chemo-electrical properties: By Vincenzo Esposito**
Period: 2 Jun 2016
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
Invited Talk - Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices 2 symposium at the 229th ECS mtg.
Links:
http://ma.ecsdl.org/content/MA2016-01/30/1496.abstract

**Related event**

**The 229th ECS Meeting**
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

**Hydrides as Energy Materials**
Period: 2 Jun 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Solid-State Lithium-Sulfur Batteries Based on Nano-Confined LiBH4

Oral Presentation

**Related event**

**Hydrides as Energy Materials: HydEM 2016**
01/06/2016 → 03/06/2016
Aarhus, Denmark
Activity: Talks and presentations › Conference presentations
Integrated Computational and Experimental Design of Next-Generation Battery Materials
Period: 1 Jun 2016 → 3 Jun 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

01/06/2016 → 03/06/2016
Aarhus, Denmark
Activity: Talks and presentations › Conference presentations

The 229th ECS Meeting
Period: 29 May 2016 → 2 Jun 2016
Heine Anton Hansen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
Oral talk: "ORR Activity of Pristine Graphite|Fe3c Interfaces"

Related event

The 229th ECS Meeting
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

The 229th ECS Meeting
Period: 29 May 2016 → 2 Jun 2016
Vladimir Tripkovic (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
Tailoring the performance of oxides for the oxygen evolution reaction

Related event

The 229th ECS Meeting
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

Lithium-Sulfur Solid-State Batteries Based on Nanoconfined LiBH4
Period: 24 May 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
2nd Cracow’s meeting on concepts related to energy
24/05/2016 → 25/05/2017
Cracow, Poland
Activity: Talks and presentations › Conference presentations

9th European Heat Pump Forum
Period: 18 May 2016 → 20 May 2016
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities
Description
Participated in the 9th EHPA forum held in Paris, France.
9th European Heat Pump Forum

Related event
9th European Heat Pump Forum
18/08/2016 → 20/08/2016
Paris, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

2016 E-MRS Spring Meeting and Exhibit
Period: 2 May 2016 → 6 May 2016
Rune E. Johnsen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Imaging and Structural Analysis
Description
Title: Micro-battery cells for detailed in situ X-ray diffraction studies of electrode materials in working metal-ion batteries
2016 E-MRS Spring Meeting and Exhibit
02/05/2016 → 06/05/2016
Lille, France
Activity: Talks and presentations › Conference presentations

Solid Oxide Fuel Cells at DTU Energy – From fundamental research towards application for renewable energy systems
Period: Apr 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related event
Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Shanghai, China
Activity: Talks and presentations › Conference presentations

Large scale heat pumps as a link between intermittent electrical energy sources and district heating sector
Period: 20 Apr 2016
Dominik Franjo Dominkovic (invited speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related event

22nd International Trade Fair and Congress for Heating,  Cooling and CHP
19/04/2016 → 21/06/2016
Frankfurt/Main, Germany
Activity: Talks and presentations › Conference presentations

Introduction to DTU Energy Research
Period: 8 Apr 2016
Søren Linderoth (Participant)
Department of Energy Conversion and Storage

Description
DTU Visit - SICCAS and SINAP/China, about SOFC research

Related event

Introduction to DTU Energy Research
08/04/2016 → 08/04/2016
Shanghai, China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
Period: 8 Apr 2016 → 11 Apr 2016
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Description
Energy Conversion Technology Development at DTU Energy

Related event

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Jiangsu, China
Activity: Talks and presentations › Conference presentations

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
Period: 8 Apr 2016 → 11 Apr 2016
Ming Chen (Organizer)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Chairman
Links:
http://www.energy.dtu.dk/english/News/Nyhed?id=d4f4b6e9-6e62-42b0-aacf-87c29a1ad8da

Related event

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Shanghai, China
Activity: Attending an event › Participating in or organising a conference

Hydrogen Day 2016
Period: 6 Apr 2016 → 8 Apr 2016
Qingfeng Li (Participant)
Department of Energy Conversion and Storage

Proton conductors

Description
Invited talk
Documents:
Abstract CISTEM Symposium 6-8 April 2016, Prague

Related event

Hydrogen Day 2016: 7th International Conference on Hydrogen Technologies
06/04/2016 → 08/04/2016
Prague, Czech Republic
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Computational Design of Materials Atomic-scale modeling of electrode reactions in Zn-air batteries
Period: 4 Apr 2016 → 6 Apr 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

1st International Zinc-Air Battery Workshop
04/04/2016 → 06/04/2016
Ulm, Germany
Activity: Talks and presentations › Conference presentations

Challenges in Going from 2nd Order to 1st Order Materials in Magnetic Refrigeration Devices
Period: 28 Mar 2016 → 1 Apr 2016
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

2016 MRS Spring Meeting
28/03/2016 → 01/04/2016
Phoenix, United States
Activity: Talks and presentations › Conference presentations

Electrolysis and electrochemistry
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Interdisciplinary Block Course „Energy and Chemistry“
29/02/2016 → 04/03/2016
Karlsruhe, Germany
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

10th International Symposium "Hydrogen & Energy"
Period: 21 Feb 2016 → 26 Feb 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
LITHIUM-SULFUR ALL-SOLID-STATE BATTERIES

Oral presentation

Related event
10th International Symposium "Hydrogen & Energy"
21/02/2016 → 26/02/2016
Sendai, Japan
Activity: Talks and presentations › Conference presentations

Computational Design of Materials for Electrochemical Energy Conversion and Storage
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
10th International Symposium "Hydrogen & Energy"
21/02/2016 → 26/02/2016
Sendai, Japan
Activity: Talks and presentations › Conference presentations

Platform for smart energi, Energistyrelsen (External organisation)
Period: 15 Feb 2016 → 30 Jun 2017
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related external organisation
Platform for smart energi, Energistyrelsen
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

40th International Conference and Exposition on Advanced Ceramics and Composites
Period: 24 Jan 2016 → 29 Jan 2016
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
13th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science, and Technology

13th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science, and Technology
Links:

Related event
40th International Conference and Exposition on Advanced Ceramics and Composites: ICACC’16
24/01/2016 → 29/01/2016
Daytona Beach, FL, United States
High Pressure Synthesis of Non-precious Metal ORR Catalysts for Fuel Cells  
Period: 18 Jan 2016 → 19 Jan 2016  
Qingfeng Li (Invited speaker)  
Department of Energy Conversion and Storage  
Proton conductors  

Description  
Invited speaker  
Documents:  
Abstract on NPMC submitted to 1st Curtin-UQ Workshop 18-19 Jan 2016  

Related event  
Curtin - University of Queensland Workshop on Nanostructured Electromaterials for Energy  
18/01/2016 → 19/01/2016  
Perth, Australia  
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities  

24th International Materials Research Congress  
Period: 2015  
Henrique Neves Bez (Speaker)  
Department of Energy Conversion and Storage  
Electrofunctional materials  

Related event  
24th International Materials Research Congress  
16/08/2015 → 20/08/2015  
Cancun, Mexico  
Activity: Talks and presentations › Conference presentations  

Annual Meeting of the Danish Electrochemical Society 2015  
Period: 2015  
Yang Hu (Speaker)  
Department of Energy Conversion and Storage  
Proton conductors  

Description  
Encapsulation structure for oxygen reduction: a preliminary understanding  
Annual Meeting of the Danish Electrochemical Society 2015  

Related event  
Annual Meeting of the Danish Electrochemical Society 2015  
01/10/2015 → 02/10/2015  
Copenhagen, Denmark  
Activity: Talks and presentations › Conference presentations  

Chemical Engineering Journal (Journal)  
Period: 2015  
Anke Hagen (Reviewer)  
Department of Energy Conversion and Storage  
Applied Electrochemistry
Related journal

Chemical Engineering Journal
1385-8947
Central database
Activity: Research › Peer review of manuscripts

Delft Days on Magnetocalorics 2015
Period: 2015
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Poster presentation

Related event

Delft Days on Magnetocalorics 2015
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

European School of Magnetism
Period: 2015 → …
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Description
From fundamental magnetism to spin currents

Related event

European School of Magnetism
24/08/2015 → 04/09/2015
Cluj-Napoca, Romania
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Fuel Cells (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Links:

Related journal

Fuel Cells
1615-6846
Central database
Activity: Communication › Journal editor

Fuel Cells (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

Fuel Cells
1615-6846
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

International Journal of Hydrogen Energy (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

International Journal of Hydrogen Energy
0360-3199
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 3.74 SJR 1.142 SNIP 1.286, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Journal of Power Sources (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

Journal of Power Sources
0378-7753
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Journal of Solid State Electrochemistry (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

Journal of Solid State Electrochemistry
1432-8488
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 2.26 SJR 0.662 SNIP 0.721, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts
PhD thesis Lisa Deleebeeck: Censor
Period: 2015
Anke Hagen (Internal examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Censor
Activity: Examinations and supervision › Internal examination

PhD thesis Olivier Thomann: Censor
Period: 2015
Anke Hagen (External examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Activity: Examinations and supervision › External examination

RFCcontrol: Open source control software for fuel cell and electrolyser test stations
Period: 2015
Søren Koch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
RFCcontrol is a generalized control system for fuel cell, electrolyser cells, battery and other types of materials test stations / test setups. It features data logging as well as device control and can handle gas flow control, temperature control, relay control, control of DC power supplies as well as handle data acquisition through a number of data logging devices.
Head: Søren Koch
Links:
http://www.rfccontrol.dk/

Related external organisation
Department of Energy Conversion and Storage
Roskilde, Denmark
Activity: Other

Study of mesoporous ZSM-5
Period: 2015 → 2016
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Diplomingeniørprojekt
Coordinated by Anke Hagen

Related external organisation
DTU Energy
Roskilde, Denmark
Activity: Other

Topics in catalysis (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

Topics in catalysis
1022-5528
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 2.55 SJR 0.974 SNIP 0.878, ISI indexed (2013): ISI indexed yes, Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts

Helmholtz Institute Ulm (External organisation)
Period: 18 Dec 2015 → …
Tejs Vegge (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Member of the International Advisory Board for Electrochemical Energy Storage, SCI Program, The Helmholtz Association
Member of the International Advisory Board for Electrochemical Energy Storage under the Program 'Storage and Cross-linked Infrastructure (SCI)'. SCI coordinates activities within at five different Helmholtz Centers, i.e. KIT, FZJ, DLR, HZB and HZDR. The topic Electrochemical Energy Storage covers the activities within electrochemical energy storage.

Body type: Advisory Board
Degree of recognition: International

Related external organisation

Helmholtz Institute Ulm
Germany
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Accelerated DFT-based Design of Materials for Ammonia Storage
Period: 15 Dec 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Links:
http://www.pacifichem.org/

Related event

PacificChem 2015
15/12/2015 → 20/12/2015
Honolulu, Hawaii, United States
Activity: Talks and presentations › Conference presentations

Nordic Battery Conference 2015
Period: 2 Dec 2015 → 3 Dec 2016
Simon Loftager (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
The Nordic Battery Conference 2015 (NordBatt 2)

Related event
Nordic Battery Conference 2015
02/12/2015 → 03/12/2015
Trondheim, Norway
Activity: Attending an event › Participating in or organising a conference

Modelling, optimisation, design and analysis of integrated energy systems
Period: 30 Nov 2015 → 4 Dec 2015
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Successfully participated in a PhD course.

"Modelling, optimisation, design and analysis of integrated energy systems" organized by EPFL, Sion, Switzerland

Related event
Modelling, optimisation, design and analysis of integrated energy systems
30/11/2015 → 04/12/2015
Sion, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Computational Design of Materials for Energy Conversion and Storage
Period: 20 Nov 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
20/11/2015 → …
Reykjavik, Iceland
Activity: Talks and presentations › Conference presentations

Gas network modelling: Master Thesis by Marco Cavana
Period: 15 Nov 2015 → 10 Jul 2016
Allan Schrøder Pedersen (Supervisor)
Centre for IT-Intelligent Energy Systems in Cities
Department of Energy Conversion and Storage
Activity: Examinations and supervision › Supervisor activities

On the Analysis of Positron Lifetime Spectra
Period: 12 Nov 2015 → 13 Nov 2015
Morten Mostgaard Eldrup (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Invited talk
Co-authors: Peter Kirkegaard and Jens V. Olsen, AIT, DTU

Related event
Tagung deutscher Positronengruppen-3
12/11/2015 → 13/11/2015
München, Denmark
Activity: Talks and presentations › Conference presentations

DFT Studies of the Oxygen Reduction Reaction on Fe3C-graphite catalysts
Period: 10 Nov 2015
Heine Anton Hansen (Keynote speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

Description
Poster presentation

Related event
08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

International Conference on Innovative Electrochemical Energy Materials and Technologies
Period: 8 Nov 2015 → 11 Nov 2015
Mateusz Reda (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Co-author of oral presentation
Related event

08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

A Perspective on Next-generation Battery Technologies
Period: 5 Nov 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Workshop on Batteries as a Game Changer?!, Intelligent Energy
05/11/2015 → …
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Delft Days on Magnetocalorics 2015
Period: 2 Nov 2015 → 3 Nov 2015
Christian Bahl (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

Delft Days on Magnetocalorics 2015
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Delft Days on Magnetocalorics 2015
Period: 2 Nov 2015 → 3 Nov 2015
Andrea Roberto Insinga (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

Delft Days on Magnetocalorics 2015
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

Danish Electrochemical Society (External organisation)
Period: 1 Nov 2015 → …
Marie Lund Traulsen (Chairman)
Department of Energy Conversion and Storage

Description
Boardmember of the Danish Electrochemical Society
Degree of recognition: National
Links:
http://www.electrochemistry.dk/
Related external organisation

Danish Electrochemical Society
Munkebjergvej 17, 4100, Ringsted, Denmark
Activity: Membership › Board duties in companies, associations, or public organisations

Descriptor based Design of Catalytic Nanoalloys and Clusters using Density Functional Theory and Genetic Algorithms
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

International Symposium on Clusters and Nanomaterials
26/10/2015 → 29/10/2015
Virginia, United States
Activity: Talks and presentations › Conference presentations

High Performance Segmented Oxides-based Materials
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

14th International Union of Materials Research Societies - International Conference on Advanced Materials
25/10/2015 → …
Activity: Talks and presentations › Conference presentations

PhD defense (opponent): Manuel Placencia Gutierez, "Searching for saddle points and global minima"
Period: 20 Oct 2015
Tejs Vegge (External examiner)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Activity: Examinations and supervision › External examination

BACHU NARAIN SINGH: ENDURING IMPACT ON RADIATION DAMAGE PHYSICS
Morten Mostgaard Eldrup (Speaker)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

Description
Talk given by 1'st author of abstract at '17th International Conference on Fusion Reactor Materials'
Participate as author

Co-authors: S.J. Zinkle1,2, M. Eldrup3, S.A. Fabritsiev4, N.M. Ghoniem5, S.I. Golubov2, H.L. Heinisch6, S. Ishino7, Yu.N. Osetsky2, and M. Victoria8
1University of Tennessee, Knoxville, TN 37996, USA
2Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
3Technical University of Denmark, Risø Campus, Roskilde, Denmark
4D.V. Efremov Scientific Research Inst., St. Petersburg, Russia
5University of California, Los Angeles, CA
6Pacific Northwest National Laboratory, Richland, WA
7University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8654, Japan
8CRPP, Villigen, Switzerland
Related event
17th International Conference on Fusion Reactor Materials
11/10/2015 → 16/10/2015
Aachen, Germany
Activity: Talks and presentations › Conference presentations

Ionic and electronic transport properties in LiFeBO₃ from DFT
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Workshop on Understanding Interfaces in Electrochemical Storage Systems
06/10/2015 → 08/10/2015
Tours, France
Activity: Talks and presentations › Conference presentations

Workshop on Understanding Interfaces in Electrochemical Storage Systems
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Workshop on understanding interfaces in electrochemical storage systems

Related event
Workshop on Understanding Interfaces in Electrochemical Storage Systems
06/10/2015 → 08/10/2015
Tours, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

The 66th Annual Meeting of the International Society of Electrochemistry
Anne Hauch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
International Society of Electrochemistry 66th annual meeting

Related event
The 66th Annual Meeting of the International Society of Electrochemistry
04/10/2015 → 09/10/2015
Taipei, Taiwan, Province of China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

ELECTROCHEMICAL CONVERSION OF CO2 INTO LIQUID FUEL ON RuO2 (110) OVERLAYERS
Period: 2 Oct 2015
Arghya Bhowmik (Lecturer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Annual Meeting of the Danish Electrochemical Society 2015
Period: 1 Oct 2015 → 2 Oct 2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Mateusz Reda (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation

Annual Meeting of the Danish Electrochemical Society 2015

Related event

Annual Meeting of the Danish Electrochemical Society 2015
Period: 1 Oct 2015 → 2 Oct 2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Description
ISOS-8
Links:

Related event

ISOS-8
Period: 1 Oct 2015
Rio de Janeiro, Brazil
Activity: Talks and presentations › Conference presentations

PhD defense (opponent): Kristian Baruel Ørnsø, "Computational design of molecules for dye sensitized solar cells and nano electronics"
Period: 1 Oct 2015
Tejs Vegge (Internal examiner)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Nye Energiteknologier: Danmarks fremtidige energisystem uden fossile brændstoffer – Brændselceller og elektrolyse
Period: Sep 2015 → Oct 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Akademiet for Talentfulde Unge.
Organizer

Related external organisation
DTU Energy
Roskilde, Denmark
Activity: Other

Polybenzimidazole membranes in alkaline water electrolysis: Chemical and electrochemical stability
Period: 29 Sep 2015 → 1 Oct 2015
Mikkel Rykær Kraglund (Other)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: International
Documents:
3DegIs poster v2

Related event
International workshop on degradation issues of fuel cells and electrolyzers
29/09/2015 → 01/10/2015
Thira, Greece
Activity: Talks and presentations › Conference presentations

Electricity Storage in Batteries
Period: 28 Sep 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Energy storage – a must for successful conversion to green energy
28/09/2015 → …
Danish Academy of Technical Sciences (ATV), Denmark
Activity: Talks and presentations › Conference presentations

Energy Supply Modelling in Cities: Illustrated Using Data from the Danish Municipality of Sønderborg
Period: 28 Sep 2015
Dadi Þorsteinn Sveinbjörnsson (Keynote speaker)
Department of Energy Conversion and Storage

Description
Session keynote presentation

Related event
Er der vedvarende energi nok til os alle?
Period: 21 Sep 2015 → 25 Sep 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Dansk Naturvidenskabsfestival 2015
21/09/2015 → 25/09/2015
Denmark
Activity: Talks and presentations › Conference presentations

4th Metal-air Workshop
Period: 14 Sep 2015 → 15 Sep 2015
Rune Christensen (Speaker)
Atomic scale modelling and materials
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design

Description
Reducing Systematic Errors in OxideSpecies with Density Functional Theory Calculations
ReLiable Metal-air battery workshop

Related event
4th Metal-air Workshop: The Road Ahead
14/09/2015 → 15/09/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

IN SITU SMALL ANGLE STUDIES OF ROLL-TO-ROLL COATED PEROVSKITE SOLAR CELLS
Period: 14 Sep 2015
Lea Hildebrandt Rossander (Speaker)
Department of Energy Conversion and Storage
Organic Energy Materials

Related event
16th Conference on Small Angle Scattering (SAS 2015)
13/09/2015 → 18/09/2015
Berlin, Germany
Activity: Talks and presentations › Conference presentations

In situ GISAXS/GIWAXS studies of roll-to-roll coated perovskite solar cells
Period: 10 Sep 2015
Lea Hildebrandt Rossander (Speaker)
Department of Energy Conversion and Storage
Organic Energy Materials
Related event

GISAS2015: 3rd International GISAS Conference
08/09/2015 → …
Nice, France
Activity: Talks and presentations › Conference presentations

PSI-K 2015 Conference
Period: 6 Sep 2015 → 10 Sep 2015
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentations: "Computational investigations of transport mechanisms across battery interfaces" and "How should the energies of localized vs. delocalized polarons be compared in supercell calculations? A case study in self-trapped polarons in silver halides"

Psi-k 2015 conference

Related event

PSI-K 2015 Conference
06/09/2015 → 10/09/2015
San Sebastian, Spain
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Energy Supply Modelling in Cities: Illustrated Using Data from the Case of Sønderborg
Period: 1 Sep 2015
Dadi Þorsteinn Sveinbjöömsson (Speaker)
Department of Energy Conversion and Storage

Related event

Nordic Climate KIC - CITIES workshop
01/09/2015 → …
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Journal of Fuel Cell Science and Technology (Journal)
Period: 1 Sep 2015 → 31 Dec 2015
Jacob R. Bowen (Editor)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Journal of Fuel Cell Science and Technology

Associate Editor

Associate Editor

Links:
http://fuelcellscience.asmedigitalcollection.asme.org (Journal of Fuel Cell Science and Technology homepage)
http://journaltool.asme.org/Content/Masthead19.cfm (Editorial Board)

Related journal

Journal of Fuel Cell Science and Technology
Novel Heterostructured and Multilayered Oxide Thin Films for Future Applications

Period: 1 Sep 2015 → 4 Sep 2015

Søren Linderoth (Keynote speaker)

Department of Energy Conversion and Storage

Related event

Donostia International Workshop on Energy Materials Nanotechnology
01/09/2015 → 04/09/2015
San Sebastian - Donostia (Guipuzcoa), Spain
Activity: Talks and presentations › Conference presentations

University of the Basque Country
Period: 1 Sep 2015 → 30 Sep 2015

Simon Loftager (Visiting researcher)

Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Description
External research stay at Nano-bio Spectroscopy Group, University of the Basque Country
Activity: Visiting an external institution › Visiting another research institution

Ionic and electronic transport in solid oxide cells – Seen from an applied perspective
Period: 25 Aug 2015

Anke Hagen (Invited speaker)

Department of Energy Conversion and Storage

Applied Electrochemistry

Related event

15th European Conference on Solid State Chemistry
23/08/2015 → 26/08/2015
Vienna, Austria
Activity: Talks and presentations › Conference presentations

European School of Magnetism
Period: 24 Aug 2015 → 4 Sep 2015

Andrea Roberto Insinga (Participant)

Department of Energy Conversion and Storage

Electrofunctional materials

Description
From fundamental magnetism to spin currents

Related event

European School of Magnetism
24/08/2015 → 04/09/2015
Cluj-Napoca, Romania
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
Materials for Energy Storage – and how DFT can improve them
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
SUNCAT Summer Institute 2015
Stanford, United States
Activity: Talks and presentations › Conference presentations

SUNCAT Summer Institute 2015
Rune Christensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation given
Summer workshop on catalysis at Stanford

Related event
SUNCAT Summer Institute 2015
Stanford, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SUNCAT Summer Institute 2015
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation: "Computational investigations of transport mechanisms across battery interfaces"
Suncat Summer Institute 2015, SLAC National Accelerator Laboratory & Stanford University

Related event
SUNCAT Summer Institute 2015
Stanford, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SUNCAT Summer Institute 2015
Mateusz Reda (Participant)
Center for Atomic-scale Materials Design
**Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries**

*Period:* 19 Aug 2015  
*Rune Christensen (Lecturer)*  
*Department of Energy Conversion and Storage*

**Description**
Lecture given while visiting Catalyst Design Lab at Brown University

**Related external organisation**
*Unknown external organisation*  
*Activity:* Talks and presentations  
*Conference presentations*

**Brown University**
*Rune Christensen (Visiting researcher)*  
*Department of Energy Conversion and Storage*

**Description**
External stay at Catalyst Design Lab  
*Activity:* Visiting an external institution  
*Visiting another research institution*

**The Danish SOC Landscape 2015**
*Period:* 1 Aug 2015  
*Anke Hagen (Invited speaker)*  
*Department of Energy Conversion and Storage*
Applied Electrochemistry

Related event

IEA Annex SOFC
01/08/2015 → 01/08/2015
Glasgow, United Kingdom
Activity: Talks and presentations › Conference presentations

On the Challenge of Stabilizing Contacts in Bi-Te Thermoelectric Generator under thermal cycling
Period: 24 Jun 2015 → 26 Jun 2015
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

Energy Harvesting Systems - FlexTEG 2015
24/06/2015 → …
Activity: Talks and presentations › Conference presentations

Atomic-scale modeling of materials for hydrogen-based energy storage
Period: 22 Jun 2015 → 26 Jun 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

4th European Technical School on Hydrogen and Fuel Cells
22/06/2015 → 26/06/2015
Crete, Greece
Activity: Talks and presentations › Conference presentations

Towards a Fossil-Free Energy System: How Possible to Achieve?
Period: 29 May 2015
Søren Linderoth (Invited speaker)
Department of Energy Conversion and Storage

Description
Clean Energy Forum: "Towards a Fossil-Free Energy System: How Possible to Achieve?"

Related event

Clean Energy Forum
29/05/2015 → …
Beijing, China
Activity: Talks and presentations › Conference presentations

Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
Period: 26 May 2015
Søren Linderoth (Invited speaker)
Department of Energy Conversion and Storage

Description
Introduction to DTU Energy
Related event

Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
Period: 26 May 2015
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

Status and Results of Energy Supply Modelling in CITIES: Illustrated using Data from the Case of Sønderborg
Period: 26 May 2015
Dadi Þorsteinn Sveinbjörnsson (Lecturer)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related event

CITIES Second General Consortium Meeting
Period: 26 May 2015
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

227th ECS Meeting
Rune Christensen (Speaker)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

Description
Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries

Speaking at and participating in 227th ECS Meeting

Related event

227th ECS Meeting
Period: 24/05/2015 → 28/05/2015
Chicago, IL, United States
Activity: Talks and presentations › Conference presentations

Vedvarende energi: Ny teknologi, der ændrer vores hverdag
Period: 20 May 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Foredrag om vedvarende energi og energikonvertering og lagring i forelæsningsserie om "Ny teknologi" på Aarhus Folkeuniversitet (Emdrup afd.)

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

PhD defense (member of evaluation committee): Edith Ahlberg Helгеe, "Significance of grain boundaries for transport phenomena in graphene and proton-conducting barium zirconate" at Chalmers University of Technology, Sweden (External organisation)
Period: 8 May 2015
Tejs Vegge (External examiner)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Activity: Examinations and supervision › External examination

Brændselceller og elektrolyse: En del af løsningen for fremtidens energiudfordringer
Period: Apr 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Public presentation: Bestil en Forsker

Related event

Bestil en forsker: Forskningens Døgn
22/04/2015 → 26/04/2015
Sønderborg, Denmark
Activity: Talks and presentations › Conference presentations

Forskningens Døgn 2015
Period: Apr 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Forskningens Døgn: Exhibition Roskilde

Related event

Forskningens Døgn 2015
22/04/2015 → 26/04/2015
Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Workshop on Advancing Caloric Materials for Efficient Cooling
Period: 29 Apr 2015
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Workshop on Advancing Caloric Materials for Efficient Cooling

Related event
Workshop on Advancing Caloric Materials for Efficient Cooling
28/04/2015 → 29/04/2015
College Park, Maryland, United States
Activity: Talks and presentations › Conference presentations

Novel electrodes for efficient and durable electrolysis and fuel cells
Period: 28 Apr 2015 → 29 Apr 2015
Peter Holtappels (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Novel electrodes for efficient and durable electrolysis and fuel cells

Related event
EERA Inter-JP cross-fertilization workshop on materials for energy applications and technologies
28/04/2015 → 29/04/2015
Brussels, Denmark
Activity: Talks and presentations › Conference presentations

3rd Conference on Frontiers of Aberration Corrected Electron Microscopy
Period: 19 Apr 2015 → 23 Apr 2015
Fabrizio Gualandris (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Poster presentation at PICO conference 2015
Degree of recognition: International
Documents:
Abstract

Related event
3rd Conference on Frontiers of Aberration Corrected Electron Microscopy
19/04/2015 → 23/04/2015
Kasteel Vaalsbroek, Netherlands
Activity: Talks and presentations › Conference presentations

Manufacturing of Green Fuels from Renewable Energy
Period: 16 Apr 2015
Arghya Bhowmik (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation on "The Influence of Electronic Structure on H/OH/CO Binding Energy on Rutile (110) Oxide Surfaces"

Related event
Manufacturing of Green Fuels from Renewable Energy
**High Temperature Alkaline Electrolysis - Progress and Potential**
Period: 15 Apr 2015
Christodoulos Chatzichristodoulou (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

**Related event**

**Manufacturing of Green Fuels from Renewable Energy**
14/04/2015 → 16/04/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Integration of improved correction schemes and operational conditions in the design of nanoalloy catalysts for CO2 reduction**
Period: 14 Apr 2015 → 16 Apr 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

**Manufacturing of Green Fuels from Renewable Energy**
14/04/2015 → 16/04/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Manufacturing of Green Fuels from Renewable Energy**
Period: 14 Apr 2015 → 16 Apr 2015
Rune Christensen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Participant and poster presenter

Workshop on Manufacturing of Green Fuels from Renewable Energy

**Related event**

**Manufacturing of Green Fuels from Renewable Energy**
14/04/2015 → 16/04/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**MRS Spring Meeting**
Period: 6 Apr 2015 → 10 Apr 2015
Qingfeng Li (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors
Iron carbide nanoparticles encapsulated by graphitic layers as ORR catalysts. Abstract on NPMC

Invited talk

Abstract on NPMC - MRS Spring Meeting, 6-10 April 2015, San Francisco, California

Related event

2015 MRS Spring Meeting & Exhibit
06/04/2015 → 10/04/2015
San Francisco, United States
Activity: Talks and presentations › Conference presentations

Design of borohydrides and novel materials for ammonia storage
Period: 18 Mar 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

IEA-teknologinetværk om brint og brændselsceller og FCH2-programmet
18/03/2015 → …
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

American Physical Society March Meeting 2015
Period: 3 Mar 2015
Kurt Engelbrecht (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Presented Invited talk titled: "Modelling and Design Aspects of Active Caloric Regenerators"

American Physical Society March Meeting
Links:
http://www.aps.org/meetings/march/index.cfm

Related event

American Physical Society March Meeting 2015
02/03/2015 → 06/03/2015
San Antonio, United States
Activity: Attending an event › Participating in or organising a conference

Asilomar 2015
Period: 10 Feb 2015
Qingfeng Li (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Description
High Temperature Durable Membranes for Fuel Cells

Invited talk
Degree of recognition: International

Abstract submitted to Advances in Polymers for Fuel Cells and Energy Devices Qingfeng Li

Related event

Asilomar 2015: Advances in Polymers for Fuel Cells and Energy Devices
08/02/2015 → 11/02/2015
Pacific Grove,, United States
Activity: Talks and presentations › Conference presentations

Energikonvertering - Brændselsceller og brint: Vedvarende Energi
Period: 10 Feb 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Forelæsning om brændselsceller og bring i forelæsningsserien ”Vedvarende Energi” på Aarhus Folkeuniversitet (Emdrup afdeling)

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

SUNCAT Center for Interface Science and Catalysis
Period: 8 Feb 2015 → 1 Mar 2015
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
External stay at SUNCAT
Stay at SUNCAT center at Stanford
Activity: Visiting an external institution › Visiting another research institution

Material & Struktur – Entscheidende Kombination für Hochtemperaturbrennstoff- und Elektrolysezellen
Period: 27 Jan 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Karlsruher Werkstoffkolloquium
27/01/2015 → ...
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations

39th International Conference and Expo on Advanced Ceramics and Composites
Period: 25 Jan 2015 → 30 Jan 2015
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
11th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology

Links:

Related event

39th International Conference and Expo on Advanced Ceramics and Composites
25/01/2015 → 30/01/2015
Daytona Beach, FL, United States
Activity: Attending an event › Participating in or organising a conference

Materials Predictors and Genetic Algorithms for Rational Design of Electro catalytic Nanoparticles
Period: 7 Jan 2015 → 11 Jan 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

9th International Conference on Computational Physics
07/01/2015 → 11/01/2015
Singapore, Singapore
Activity: Talks and presentations › Conference presentations

6th IIR/IIF International Conference on Magnetic Refrigeration
Period: 2014
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Poster presentation on thermal hysteresis of manganite

Related event

6th IIR/IIF International Conference on Magnetic Refrigeration
07/09/2014 → 10/09/2014
Victoria, Canada
Activity: Attending an event › Participating in or organising a conference

Angewandte Chemie (International Edition) (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal

Angewandte Chemie (International Edition)
1433-7851
Central database
Activity: Research › Peer review of manuscripts
Applied Catalysis A-general (Journal)
Period: 2014
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal
Applied Catalysis A-general
0926-860X
Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts

Årsmøde 2014 i Dansk Batteriselskab
Period: 2014 → …
Jonathan Højberg (Organizer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Links:
http://batteriselskab.dk/danish-battery-symposium-2014

Related event
Årsmøde 2014 i Dansk Batteriselskab
28/02/2014 → …
Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Chemical Review (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Chemical Review
Local database
Activity: Research › Peer review of manuscripts

Fuel Cells (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Fuel Cells
1615-6846
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 1.79 SJR 0.498 SNIP 0.62, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

HyFC Academy PhD Workshop on Catalysts for Fuel Cells and Electrolysers
Period: 2014
James Atwoki Mugabi (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
HyFC (The Danish Hydrogen and Fuel cell academy, 2014)

Related event
HyFC Academy PhD Workshop on Catalysts for Fuel Cells and Electrolysers
13/02/2014 → …
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Journal of Chemical Physics (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Journal of Chemical Physics
0021-9606
BFI (2018): BFI-level 2, Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Nature Chemistry (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Nature Chemistry
1755-4330
Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts

Nature Materials (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related journal**

*Nature Materials*
1476-1122
Central database
Activity: Research › Peer review of manuscripts

**Optical antennas, optical cavity and photonic crystals to enhance the performance of organic solar cells**
Period: 2014
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**E-MRS 2014 Spring Meeting**
25/05/2014 → 30/05/2014
Lille, France
Activity: Talks and presentations › Conference presentations

**QuantumHagen**
Period: 2014 → …
Rune Christensen (Participant)
Department of Energy Conversion and Storage

**Related event**

**QuantumHagen: Workshop on Modeling of Electronic Devices and Materials at the Nanoscale**
01/07/2014 → 03/07/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Referee for Netherlands Organisation for Scientific Research (NWO) - Chemical Sciences (External organisation)**
Period: 2014
Tejs Vegge (Member)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

**Related external organisation**

**Referee for Netherlands Organisation for Scientific Research (NWO) - Chemical Sciences**
Activity: Membership › Membership in review committee

**Referee for US Department of Energy (DoE), Energy Frontiers Research Centers (EFRC) (External organisation)**
Period: 2014
Tejs Vegge (Member)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Related external organisation

Referee for US Department of Energy (DoE), Energy Frontiers Research Centers (EFRC)
Activity: Membership › Membership in review committee

ReLiable Workshop III
Period: 2014
Rune Christensen (Participant)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

Related event

ReLiable Workshop III
25/08/2014 → 26/08/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Semitransparent Organic Solar Cell toward Opaque Performances
Period: 2014 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event

2014 MRS Spring Meeting
21/04/2014 → 25/04/2014
San Francisco, United States
Activity: Talks and presentations › Conference presentations

The Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal

The Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter
1932-7447
Central database
Activity: Research › Peer review of manuscripts

Elchemea Data Aquisition: Software til impedansspektroskopi, cyklisk voltametri samt chronopotentiometri/vamperometri
Period: Dec 2014
Søren Koch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Scalable Roll-to-Roll Fabrication for Fully Solution-Processed Polymer Solar Cells from Small-Scale Test Devices to Multi Square Meter Large Modules for Energy Production

Period: 3 Dec 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage

Functional organic materials

Description
The majority of lab-scale organic and polymer solar cells (OPV) are very small with $<<0.5 \text{ cm}^2$ using ITO glass, spin coating, evaporation, inert atmosphere, and optimum conditions. Obviously, the cells can lead to record efficiencies - but they are far beyond real world applications due to miniscule power output. Transfer to large-scale devices with an appropriate power output is hardly possible.

Here, we present the route from roll and roll-to-roll processed test devices to multi square meter large polymer solar cell modules with hundreds of Watts output - fully roll-to-roll (R2R) produced under vacuum-free and ambient conditions without using indium tin oxide (ITO) as transparent conductive electrode. ITO has the highest impact on the embodied energy in OPV devices and is replaced by an all additive printed and coated electrode based on flexo printed silver grid, rotary screen printed PEDOT:PSS, and slot-die coated zinc oxide (Flextrode). The production speed for each layer is beyond 10 m/min independently of the individual layout for different devices.

Model cells with at least 1 cm² are fabricated on a rollcoater, which allows easy transfer to the R2R line for larger test modules with e.g. 8 serially connected cells and the size of a postcard (freeOPV, active area $>50 \text{ cm}^2$). Both routes allow the testing of new polymers, functional inks, and device structures such as tandem stacks with minimum amount of material input but large number of devices for statistical analyses.

Finally, OPV modules with high power output for real-world applications and grid-connection can be easily produced based on the Infinity concept developed in our group. Virtually infinite large solar cell modules are based on thousands of serially connected cells entirely fabricated using very fast R2R printing and coating processes. No manual labour or proprietary processes are required for bussing and interconnection of submodules. The serial connection is completed throughout the print run due to an optimized pattern layout. The advantage of the Infinity concept is the fabrication of high-voltage OPV modules with active areas beyond several square meters (21000 cells = 14.7 m², 100 m long) and stabilized power outputs of $>220$ W using the standard active layer material P3HT:PCBM. The module has only two terminal connectors for minimized wiring during the setup of module arrays. The installation of a 100 m long module takes less than one minute. A parallel-connected array with outputs $>1.3$ kW and rather low efficient material (<2%) was built. An entire solarpark based on such OPV modules has a low energy payback time of just 0.5 years.

Related event
2014 MRS Fall Meeting & Exhibit
30/11/2014 → 05/12/2014
Boston, United States
Activity: Talks and presentations › Conference presentations

International Carisma Conference
Period: 1 Dec 2014 → 3 Dec 2014
Jens Oluf Jensen (Speaker)
Department of Energy Conversion and Storage

Proton conductors

Description

Related event
International Carisma Conference
**2014 MRS Fall Meeting & Exhibit**  
**Period:** 30 Nov 2014 → 5 Dec 2014  
**Simona Ovtar (Participant)**  
Department of Energy Conversion and Storage  
**Mixed Conductors**  
**Description**  
Enhanced oxygen exchange of \( \text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_{3-\delta} - \text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95} \) composites  
**Documents:**  
abstract  
**Related event**  
**2014 MRS Fall Meeting & Exhibit**  
30/11/2014 → 05/12/2014  
Boston, United States  
**Activity:** Attending an event › Participating in or organising workshops, courses, seminars etc.  

**Conference on Energy and Environment for the Future**  
**Period:** 24 Nov 2014 → 25 Nov 2014  
**Emil Bøje Lind Pedersen (Speaker)**  
Imaging and Structural Analysis  
Department of Energy Conversion and Storage  
**Description**  
Presented a poster titled: “Ptychographic Tomography of an organic tandem solar cell”.  
Participated in "Energy and Environment for the future".  
**Related event**  
**Conference on Energy and Environment for the Future: Sustainable energy for a fossil free society and environmentally friendly technologies**  
Copenhagen, Denmark  
**Activity:** Talks and presentations › Conference presentations  

**Conference on Energy and Environment for the Future**  
**Period:** 24 Nov 2014 → 25 Nov 2014  
**Jens Oluf Jensen (Speaker)**  
Department of Energy Conversion and Storage  
**Proton conductors**  
**Description**  
**Related event**  
**Conference on Energy and Environment for the Future: Sustainable energy for a fossil free society and environmentally friendly technologies**  
Copenhagen, Denmark  
**Activity:** Talks and presentations › Conference presentations
Børnenes Universitet 2014
Period: 22 Nov 2014
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Børnenes Universitet: Workshop Vi fanger Solen

Related event

Børnenes Universitet 2014
22/11/2014 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Andet symposium hos Institut for Energikonvertering- og lagring
Period: 21 Nov 2014
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Physics
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Andet symposium hos Institut for Energikonvertering- og lagring
21/11/2014 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Positron Annihilation Spectroscopy on LIBH4 and LIBH4:LiI superionic lithium conductors
Period: 13 Nov 2014
Morten Mostgaard Eldrup (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Documents:
Eldrup_PPC11-abstractX
Eldrup_PPC11_abstractX.pdf
Links:
http://www.barc.gov.in/symposium/ppc11/

Related event

11th International Workshop on Positron and Positronium Chemistry
09/11/2014 → 14/11/2014
Goa, India
Activity: Talks and presentations › Conference presentations

Overpotentials and Transport Mechanisms in Metal-air Batteries
Period: 12 Nov 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Related event

EEWS Workshop: Advanced Technology for Next Generation Energy Storage System
12/11/2014 → …
Daejeon, Korea, Republic of
Activity: Talks and presentations › Conference presentations

Symposium on Nanoscale Thermal Transport
Period: 10 Nov 2014
Kaspar Kirstein Nielsen (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Nanothermal transport

Related event

Symposium on Nanoscale Thermal Transport
10/11/2014 → 10/11/2014
Gothenburg, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

High temperature electrolysis activities at Technical University of Denmark
Period: 7 Nov 2014
Sune Dalgaard Ebbesen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Documents:
leafletfuelcells-3

Related event

Fuel Cells & Electrolysers Energy for the future
07/11/2014 → …
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

The Needs for Storage/Flexibility in the Danish Energy System: Drivers, application areas and requirements
Period: 5 Nov 2014
Allan Schrøder Pedersen (Lecturer)
Department of Energy Conversion and Storage

Description
An overview of expected need for energy storage in the future Danish energy system was given in collaboration with Energinet.dk. In addition recommended storage technologies relevant in a Danish context were pointed out.

Presentation given in collaboration with Energinet.dk

Related event

European Utility Week
04/11/2014 → 06/11/2014
Amsterdam, Netherlands
Activity: Talks and presentations › Conference presentations
**Metal-air Batteries: Fundamental Mechanisms and Limitations**  
*Period:* 4 Nov 2014 → 6 Nov 2014  
Tejs Vegge (Invited speaker)  
Center for Atomic-scale Materials Design  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials

**Related event**

**Materials for Tomorrow**  
04/11/2014 → 06/11/2014  
Gothenburg, Sweden  
Activity: Talks and presentations › Conference presentations

**Optimization model for transportation fuels and SNG production from renewable sources in Denmark: Master Thesis**  
**Alessia Elia**  
*Period:* 1 Nov 2014 → 1 Jul 2015  
Allan Schrøder Pedersen (Supervisor)  
Centre for IT-Intelligent Energy Systems in Cities  
Department of Energy Conversion and Storage  
**Description**  
The purpose of this Master Thesis was to create an optimization tool for the analysis of fuels production for transportation and SNG1 for residential and industrial sectors using renewable energy. The system analyzed is mainly focused on the possible paths to obtain fuels using biomass and hydrogen (produced using electrolysis) as input and all the connections to combine these resources and energy vector in the best way. After a brief introduction and theoretical presentation, in chapter 3 the system analyzed is explained and the model is developed. In Chapter 4 the data and values adopted in the model are presented. The model is designed to minimize the breakeven cost of the system satisfying the energy demand. Finally, a wide category of scenarios were run, each distinguished by different choices of energy demand or technology processes. In the end, some of these scenarios were performed in sensitivity analyses regarding the amount of energy resources, their price, and the obligations of production using certain pathways. The model gives the possibility to investigate different parameters but results obtained were mainly focused about the amount of energy inputs consumed and the break-even cost. For each analysis the solver computes a meaningful solution which suggests different combination of energy inputs and technology to use.  
Activity: Examinations and supervision › Supervisor activities

**Magnetic Materials and Applications seminar**  
*Period:* 28 Oct 2014 → Dec 2014  
Christian Bahl (Participant)  
Department of Energy Conversion and Storage  
Electrofunctional materials

**Related event**

**Magnetic Materials and Applications seminar**  
28/10/2014 → 29/10/2014  
Lucerne, Switzerland  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**International Conference on X-Ray Microscopy**  
*Period:* 26 Oct 2014 → 31 Oct 2014  
Emil Bøje Lind Pedersen (Speaker)  
Imaging and Structural Analysis  
Department of Energy Conversion and Storage
Description
Presented a poster titled: "Ptychographic Tomography of an Organic Tandem Solar Cell Containing Active Layers Cast from Solution and Water-Dispersable Nano Particles"

Poster presentation at XRM (International X-Ray Microscopy Conference 2014)

Related event

International Conference on X-Ray Microscopy
26/10/2014 → 31/10/2014
Melbourne, Australia
Activity: Talks and presentations › Conference presentations

Solid oxide cells: Smart electrochemical devices for the smart energy systems of the future
Period: 22 Oct 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Colloquium Next Energy
22/10/2014 → …
Oldenburg, Germany
Activity: Talks and presentations › Conference presentations

Period: 14 Oct 2014
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Materials Science & Technology 2014
Links:

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

The Focused Ion Beam – Scanning Electron Microscope: A tool for sample preparation, two and three dimensional imaging
Period: 13 Oct 2014
Jacob R. Bowen (Guest lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Remote teaching guest lecture (2 hours) as part of The Univerity of Connecticut course: ME3295/5895 Three Dimensional Imaging of Materials

Guest lecturer

Slides available on request
Links:
http://www.engr.uconn.edu/me/cms/people/39-wilsonchiu (Website of Prof. Wilson K.S. Chiu (Course co-ordinator))
**Related external organisation**

**University of Connecticut**

United States

Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

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**ISOS-7**

Period: 7 Oct 2014

Michael Corazza (Speaker)

Department of Energy Conversion and Storage

**Description**

International Summit in OPV Stability (ISOS 7)

**Links:**
https://www.youtube.com/watch?v=TCUMDi7yM5v0&feature=youtu.be&list=PLav_yj0i6GkylvM4c92qdqt212rFYKYtORh

**Related event**

**ISOS-7**

06/10/2014 → 08/10/2014

Barcelona, Spain

Activity: Talks and presentations › Conference presentations

**A Stability Study of Alkali Doped PBI Membranes for Alkaline Electrolyzer Cells**


Jens Oluf Jensen (Invited speaker)

Department of Energy Conversion and Storage

**Proton conductors**

**Related event**

**226th Meeting of the Electrochemical Society (ECS) and 7th Meeting of the Mexico Section of the Electrochemical Society ECS and SMEQ Joint International Meeting : Joint international meeting**

05/10/2014 → 09/10/2014

Cancun, Mexico

Activity: Talks and presentations › Conference presentations

**HIGH TEMPERATURE ALKALINE ELECTROLYSIS**

Period: 2 Oct 2014

Christodoulos Chatzichristodoulou (Lecturer)

Department of Energy Conversion and Storage

**Fundamental Electrochemistry**

**Documents:**

HIGH TEMPERATURE ALKALINE ELECTROLYSIS_abstract

**Related external organisation**

**Unknown external organisation**

Activity: Talks and presentations › Conference presentations

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**Er der vedvarende energi nok til os alle?: Om brændselsceller og elektrolyseceller til effektiv energikonvertering**

Period: 26 Sep 2014

Anne Hauch (Lecturer)

Department of Energy Conversion and Storage

**Applied Electrochemistry**
**Description**
Foredrag i forbindelse med Dansk Naturvidenskabsfestival

Inviteret foredrag
Documents:
Brændselsceller_og_elektrolyseceller_DanskNaturvidenskabsfestival_AnneHauch_September26th2014

**Related event**

**Dansk Naturvidenskabsfestival**
26/09/2014 → …
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Atomic-scale modeling in fuel cell, electrolyser and battery research; Transport modeling in batteries -ionic and electronic transport; Beyond Li-ion - resource-efficient batteries
Period: 22 Sep 2014 → 26 Sep 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

**JESS Summer School**
22/09/2014 → 26/09/2014
Crete, Greece
Activity: Talks and presentations › Conference presentations

Massive scale production and installation of flexible printed solar cells
Period: 19 Sep 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**EOS Annual Meeting 2014 (EOSAM)**
15/09/2014 → 19/09/2014
Berlin Adlershof, Germany
Activity: Talks and presentations › Conference presentations

Solid State Protonic Conductors - 17
Period: 14 Sep 2014 → 19 Sep 2014
Jens Oluf Jensen (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

**Description**
One great advantage of the most common fuel cells, the polymer based fuel cells, is the low operating temperature which allows for easy and fast start-up and a variety of materials for construction and sealing. However, over the years the interest for increasing the working temperature has been growing. The motivation is diverse. A slight increase above 100-120°C is desired by the automotive industry to ease thermal control. This has been attempted via optimization of the perfluorosulphonic acid based membranes. A further increase to 140-200°C is desired to increase the tolerance to CO and thus to ease the integration with a reformer for carbonaceous fuels. This has been achieved by the phosphoric acid doped polymer membranes like polybenzimidazole with the added benefit that water management is unnecessary. The next step in temperature could be to go above 230-250°C in order to utilize the waste heat for methanol steam reforming. This is most realistic with solid inorganic proton conductors or molten salts and phosphate systems like CsH2PO4 have proven promising. At even higher temperature reforming of dimethyl ether and after that ethanol should be possible. Another advantage of increased temperature might be that a candidate for replacing platinum as catalyst is more easily found.
From the other end of the fuel cell temperature window solid oxide fuel cells are developing in the direction of lower operating temperatures from initially 1000°C to 600-700°C or even lower. The limiting factor is oxide ion conductivity, but which temperature would ultimately be the optimum if one could choose freely? The presentation will elaborate on the benefits of the different working temperatures based on simple system requirements with and without fuel reformers. Overall criteria are energy efficiency and system simplicity.


Related event

Solid State Protonic Conductors - 17
14/09/2014 → 19/12/2014
Seoul, Korea, Republic of
Activity: Talks and presentations › Conference presentations

18th International Microscopy Congress
Period: 10 Sep 2014
Jacob R. Bowen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Microstructure analysis of vacuum plasma sprayed electrodes for alkaline electrolysis Oral presentation of abstract MS-14-O2142

Related event

18th International Microscopy Congress 2014
07/09/2014 → 12/09/2014
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

Future Challenges for Room Temperature AMR Devices
Period: 10 Sep 2014
Kurt Engelbrecht (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

6th IIR/IIF International Conference on Magnetic Refrigeration
07/09/2014 → 10/09/2014
Victoria, Canada
Activity: Talks and presentations › Conference presentations

Design and Initial Testing of a Compact and Efficient Rotary AMR Prototype
Period: 8 Sep 2014
Dan Eriksen (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
6th IIR/IIF International Conference on Magnetic Refrigeration
Period: 7 Sep 2014 → 10 Sep 2014
Christian Bahl (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
6th IIR/IIF International Conference on Magnetic Refrigeration
Period: 7 Sep 2014 → 10 Sep 2014
Victoria, Canada
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

International Summer School on OPV
Period: 4 Sep 2014
Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Description
Presentation of a poster

International summer school on OPV
Documents:
Program summer school RHIN-SOLAR 2014
Poster_strasburg

Related event
International Summer School on OPV
31/08/2014 → 04/09/2014
Strasbourg, France
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

DTU Energy Conversion 2nd International PhD Summer School
Period: 29 Aug 2014
Jacob R. Bowen (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
The focused ion beam scanning electron microscope (FIB-SEM) is a versatile microscope that can be used for a wide range of applications including site specific transmission electron microscope (TEM) sample preparation, ion beam lithography, micro machining, integrated circuit edits, cross-sectioning and for serial sectioning to generate high resolution three dimensional images of microstructure. In the past decade the FIB-SEM has enabled many critical investigations of electrode microstructure to be performed. Electrodes tend to be made from heterogeneous stochastic porous composite materials that often have important nanoscale microstructure features. Making TEM samples to reveal critical local information from active sites within these electrodes is challenging. The FIB-SEM’s ability to make site specific samples regardless of material composition and hardness has been a major breakthrough for these devices. The FIB-SEM has also opened the door to nanometer resolution 3D imaging of electrode microstructures and provided access to for the first time microstructure parameters of electrodes only obtainable from 3D data. This talk will cover ion beam and FIB column basics, interactions of ions with materials for producing images and sputtering, ion and electron beam induced chemical vapour deposition, advantages and disadvantages of TEM sample preparation, practical aspects of serial sectioning for SEM imaging and electron backscatter diffraction (EBSD) from the users point of view. A series of examples of TEM sample preparation, 3D reconstructions and 3DEBSD on a range of energy materials will be presented as well as the
range of information that can be extracted from 3D reconstructions of electrodes.

The Focused Ion Beam – Scanning Electron Microscope: A tool for sample preparation, two and three dimensional imaging

Course lecturer
Documents:
2014 IMAGINE FIB-SEM JR Bowen
Links:
https://files.conferencemanager.dk/medialibrary/010c1367-e991-4a33-ab10-1953247e9c23/images/2014_IMAGINE_FIB-SEM_JR_Bowen.pdf (Link to slides on summer school website)
http://www.conferencemanager.dk/IMAGINE/imagine.html (Summer school website)

Related event

25/08/2014 → 29/08/2014
Hundested, Denmark
Activity: Other

Kristine Munk Jespersen (Participant)
Department of Wind Energy
Composites and Materials Mechanics
Department of Energy Conversion and Storage

Description
Participation in DTU Energy Conversion 2nd International PhD Summer School along with poster presentation. The poster has been attached to this description.

Documents:
IMAGINE Poster by kmun

Related event

DTU Energy Conversion 2nd International PhD Summer School
Hundested, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Janet Jonna Bentzen (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Documents:
abstract_IMAGINE_jabe
IMAGINE_poster_jabe

Related event

DTU Energy Conversion 2nd International PhD Summer School
Hundested, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
**International Conference on SINTERING 2014**


Francesca Teocoli (Participant)

Department of Energy Conversion and Storage

Ceramic Engineering & Science

**Description**

SINTERING 2014 continues the series of sintering conferences which have previously been held in Pennsylvania, USA (1995, 1999, 2003), Grenoble, France (2005), California, USA (2008) and last time in Jeju, Korea (2011). The International Conference on SINTERING 2014 deals with the latest developments in the field of sintering. Advances in sintering theory, modelling and the sintering of all classes of powder materials from experimental to industrial scale are considered. We are looking forward to presentations and discussions in the following fields of expertise in particular • Fundamental Aspects of Sintering • Modelling and Simulation • Multi-Material Systems • Microstructure and Properties • Novel Sintering Processes • Sintering of Nano-structured Materials • Functional Materials • Chemical Interactions during Sintering • In-situ Measurement

**Documents:**

Abstract - Sintering2014
Links:
http://www.sintering2014.com

**Related event**

**International Conference on SINTERING 2014**

24/08/2014 → 28/08/2014

Dresden, Germany

Activity: Attending an event › Participating in or organising a conference

**Magnetocaloric Cooling and Heating**

Period: 22 Aug 2014

Søren Linderoth (Lecturer)

Department of Energy Conversion and Storage

**Description**

Invited to Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science

**Documents:**

Prof Linderoth-Poster

**Related event**

**Seminar at Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science**

22/08/2014 → …

Beijing, China

Activity: Talks and presentations › Conference presentations

**Academic research in higher education**

Period: 20 Aug 2014

Duc-The Ngo (Invited speaker)

Department of Energy Conversion and Storage

Imaging and Structural Analysis

Department of Micro- and Nanotechnology

Molecular Windows

**Description**

A keynote lecture at Vietnam Summer School of Science

Vietnam Summer School of Science
Related external organisation

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

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**5th International Conference on Ceramics**
Søren Linderoth (Keynote speaker)
Department of Energy Conversion and Storage

**Description**
Professor Søren Linderoth was a keynote speaker at the ICC5 in Beijing, China, August 2014

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**5th International Conference on Ceramics: ICC5**
18/08/2014 → 22/08/2014
Beijing, China
Activity: Talks and presentations › Conference presentations

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**2014 CAMD Summer School on Electronic Structure Theory and Materials Design**
Rune Christensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

**Description**
CAMD Summer School

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**2014 CAMD Summer School on Electronic Structure Theory and Materials Design**
17/08/2014 → 23/08/2014
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

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**Electrochemical Energy Storage and Electrofuels**
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

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**Related event**

**Electrochemical Energy Storage and Electrofuels**
17/08/2014 → 23/08/2014
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

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**14th International Symposium on Metal-Hydrogen Systems: Fundamentals and Applications**
Period: 22 Jul 2014
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Poster presentation - A Class of Superior Ammonia Storage Materials Based on Solid Solution of Barium Strontium Chloride Salts Got a poster award.

Related event

14th International Symposium on Metal-Hydrogen Systems: Fundamentals and Applications
20/07/2014 → 25/07/2014
Manchester, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Board Committee Member of The International Academy of Electrochemical Energy Science (External organisation)
Period: 14 Jul 2014 → 14 Jul 2017
Qingfeng Li (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
The International Academy of Electrochemical Energy Science

Body type: an international organization
Degree of recognition: International

Related external organisation

Board Committee Member of The International Academy of Electrochemical Energy Science
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

13th International Conference Inorganic Membranes
Period: 8 Jul 2014
Shiyang Cheng (Speaker)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Best student poster award

Related event

13th International Conference Inorganic Membranes
06/07/2012 → 09/07/2014
Brisbane, Australia
Activity: Talks and presentations › Conference presentations

Overview of SOFC/SOEC development at DTU Energy Conversion
Period: 2 Jul 2014
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

European fuel cell 2014 - 11th European SOFC and SOE Forum 2014
01/07/2014 → 04/07/2014
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations
Designing Nanoparticle Electrocatalysts for Sustainable Production of Synthetic Fuels
Period: 1 Jul 2014 → 3 Jul 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
QuantumHagen: Workshop on Modeling of Electronic Devices and Materials at the Nanoscale
01/07/2014 → 03/07/2014
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

European fuel cell 2014 - 11th European SOFC and SOE Forum 2014
Period: 1 Jul 2014 → 4 Jul 2014
Benoit Charlas (Participant)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Poster B1107 - Residual stresses in a co-sintered SOC half-cell during post-sintering cooling
European Fuel cell forum 2014

Related event
European fuel cell 2014 - 11th European SOFC and SOE Forum 2014
01/07/2014 → 04/07/2014
Lucerne, Switzerland
Activity: Attending an event › Participating in or organising a conference

European fuel cell 2014 - 11th European SOFC and SOE Forum 2014
Period: 1 Jul 2014 → 4 Jul 2014
Anne Hauch (Speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
"Ni/YSZ microstructure optimization for long-term stability of solid oxide electrolysis cells" (presentation)

Related event
European fuel cell 2014 - 11th European SOFC and SOE Forum 2014
01/07/2014 → 04/07/2014
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations

QuantumWise Workshop
Period: 1 Jul 2014 → 3 Jul 2014
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Related event

QuantumWise Workshop
01/07/2014 → …
København, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Period: Jun 2014
Ngo Van Nong (Chairman)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Oxide devices: thermoelectric conversion, Resistive sensors, spintronics, and superconductors

10/06/2014 → …
Taipei, Taiwan, Province of China
Activity: Attending an event › Participating in or organising a conference

IUMRS-ICEM 2014
Period: Jun 2014
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Thermoelectric oxides for effective power generation from high temperature waste heat

Unknown external organisation
Activity: Talks and presentations › Conference presentations

International Conference on Synthetic Metal
Period: 30 Jun 2014 → 5 Jul 2014
Emil Bøje Lind Pedersen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Participated with a talk titled: "Characterization of organic water dispersible nanoparticles useable in photovoltaics"

Talk at ICSM 2014 (International Conference on Synthetic Metals)

International Conference on Synthetic Metal: Synthetic Metals Guiding the Future
30/06/2014 → 05/07/2014
Turku, Finland
Activity: Talks and presentations › Conference presentations

In situ and operando X-ray absorption spectroscopy on SOFC materials and cells
Period: 27 Jun 2014
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Challenges and Opportunities in In Situ Studies of Solid Oxide Electrodes
26/06/2014 → 27/06/2014
Risø, Denmark
Activity: Talks and presentations › Conference presentations

ASME 2014 12th Biennial Conference on Engineering Systems Design and Analysis
Kurt Engelbrecht (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Track co-leader Heat Transfer and Thermal Engineering

Session chair: Numerical Applications 1
Gave presentation: "Modelling and Simulation of Regenerators With Complex Flow Arrangements for Active Magnetocaloric Refrigeration"

Related event

ASME 2014 12th Biennial Conference on Engineering Systems Design and Analysis
Period: 25/06/2014 → 27/06/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Computational Search for Improved Ammonia Storage Materials
Period: 19 Jun 2014
Peter Bjerre Jensen (Lecturer)
Atomic scale modelling and materials
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design
Department of Physics
Documents:
abstract

Related event

CIMTEC 2014: 6th Forum on New Materials
15/06/2014 → 19/06/2014
Montecatini Terme, Italy
Activity: Talks and presentations › Conference presentations

CIMTEC 2014
Period: 18 Jun 2014
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Presentation title: Mixed Metal Ammine Complexes for Hydrogen/NH3 Storage

Oral presentation
Materials Predictors and Genetic Algorithms for Rational Design of Electrocatalytic Nanoclusters
Period: 16 Jun 2014 → 21 Jun 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

20th World Hydrogen Energy Conference 2014
Period: 15 Jun 2014 → 20 Jun 2014
Jens Oluf Jensen (Speaker)
Department of Energy Conversion and Storage
Proton conductors

Description

Danscatt Annual Meeting 2014
Period: 22 May 2014 → 23 May 2014
Emil Beje Lind Pedersen (Speaker)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
Presented a poster titled: "X-ray study of organic nanoparticles for plastic solar cells"

Participation in "Danscatt Annual Meeting 2014"
Designing New Materials for Ammonia Storage Using Density Functional Theory and Genetic Algorithms
Period: 14 May 2014
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design
Atomic scale modelling and materials
Documents:
A-O- 099 - Jensen Peter Bjerre

Related event
International Discussion on Hydrogen Energy and Applications
12/05/2014 → 14/05/2014
Nantes, France
Activity: Talks and presentations › Conference presentations

QENS 2014 / WINS 2014
Period: 13 May 2014
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Presentation title: Li-ion conduction in the LiBH4:LiI system from density functional theory calculations and quasi-elastic neutron scattering
Oral Presentation

Related event
QENS 2014 / WINS 2014
11/05/2014 → 16/05/2014
Autrans, France
Activity: Talks and presentations › Conference presentations

Will organic photovoltaic technology render benefits in a near future of a 30 years horizon?
Period: 12 May 2014
Nieves Espinosa Martinez (Lecturer)
Department of Energy Conversion and Storage
Functional organic materials

Related event
SETAC Europe 24th Annual Meeting
11/05/2014 → 15/05/2014
Basel, Switzerland
Activity: Talks and presentations › Conference presentations

Brændselsceller og elektrolyse: En del af løsningen for fremtidens energiudfordringer
Period: Apr 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Four public presentations: Roskilde Gymnasium, Helsingør Technical Museum, Kirke Helsinge Skole, Nordstjerneskolen Helsinge
Related event

Bestil en Forsker - Forskningens Døgn
24/04/2014 → 26/04/2014
Denmark
Activity: Talks and presentations › Conference presentations

Forskningens Døgn 2014
Period: Apr 2014
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Forskningens Døgn 2014
24/04/2014 → 24/04/2014
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Infinitely Large Organic Solar Cell Modules: At The Edge Of Traditional Territories For Power Supply
Period: 16 Apr 2014
Nieves Espinosa Martinez (Invited speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event

2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
Activity: Talks and presentations › Conference presentations

Fully printed multi square meter large organic solar cell modules for real energy production
Period: 15 Apr 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event

2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
Activity: Talks and presentations › Conference presentations

Outdoor Operational Stability of Indium-free Polymer Solar Cell Modules Investigated over 1 year
Period: 15 Apr 2014
Dechan Angmo (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event

2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
IRENA Workshop - The Transformative Power of Storage: Developing IRENA's Electricity Storage Roadmap
Period: 27 Mar 2014
Allan Schrøder Pedersen (Lecturer)
Department of Energy Conversion and Storage

Description
An overview of energy storage technology development roadmap work done in a European and Danish perspective was given. Presentation given in collaboration with Energinet.dk.

Related event
IRENA Workshop: The Transformative Power of Storage: Developing IRENA's Electricity Storage Roadmap
27/03/2014 → …
Düsseldorf, Denmark
Activity: Talks and presentations › Conference presentations

What is a solar cell
Period: 27 Mar 2014
Michael Corazza (Lecturer)
Department of Energy Conversion and Storage
Functional organic materials
Documents:
Program 27 3 HTX Roskilde- intro
What is a Solar Cell_v3

Related event
High school talk
27/03/2014 → 27/03/2014
Denmark
Activity: Talks and presentations › Conference presentations

Department of Energy Conversion and Storage-Solid Oxide Fuel and Electrolysis Cells
Period: 12 Mar 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Department of Energy Conversion and Storage-Solid Oxide Fuel and Electrolysis Cells
12/03/2014 → …
Lund, Sweden
Activity: Talks and presentations › Conference presentations

Dansk energisystem uden fossile brændsler – er det muligt?
Period: 6 Mar 2014
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Related event
Møde i UNF København (Ungdommens Naturvidenskabelige Forening)
06/03/2014 → …
København, Denmark
Activity: Talks and presentations › Conference presentations
Computational of Nanoparticle Catalysts for Sustainable Production of Synthetic Fuels
Period: 16 Feb 2014 → 21 Feb 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
8th International Symposium Hydrogen and Energy
16/02/2014 → 21/02/2014
Zhaoqing, China
Activity: Talks and presentations › Conference presentations

High resolution ptychographic tomography of soft matter
Period: 30 Jan 2014
Jens Wenzel Andreasen (Invited speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Links:
https://indico.desy.de/getFile.py/access?resId=47&amp;materialId=0&amp;confId=9088 (Programme)

Related event
4th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III: DESY Photon Science Users' Meeting
29/01/2014 → 31/01/2014
Hamburg, Germany
Activity: Talks and presentations › Conference presentations

Mechanical Properties of Ceramics and Glass
Period: 30 Jan 2014 → 31 Jan 2014
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Short Course: Mechanical Properties of Ceramics and Glass. Instructors: Richard C. Bradt, University of Alabama, and George Quinn, NIST

Participation to the short course on "Mechanical Properties of Ceramics and Glass".

Related event
Mechanical Properties of Ceramics and Glass
30/01/2014 → 31/01/2014
Daytona Beach - Florida, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

38th International Conference and Expo on Advanced Ceramics and Composites
Period: 26 Jan 2014 → 31 Jan 2014
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
**Description**
11th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology

38th International Conference and Expo on Advanced Ceramics and Composites

Links:

**Related event**

38th International Conference and Expo on Advanced Ceramics and Composites
26/01/2014 → 31/01/2014
Daytona Beach, FL, United States
Activity: Attending an event › Participating in or organising a conference

**Thermo-mechanical properties of SOFC components investigated by a combined method**
Period: 26 Jan 2014
Francesca Teocoli (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
Abstract_ICACC14_Teocoli_Francesca

**Related event**

38th International Conference and Exposition on Advanced Ceramics and Composites
26/01/2014 → 31/01/2014
Daytona Beach, FL, United States
Activity: Talks and presentations › Conference presentations

**Eurotech participants meeting**
Period: 23 Jan 2014
Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials
Documents:
140124 - EuroTech - Summary

**Related event**

Eurotech participants meeting
23/01/2014 → 24/01/2014
Neuchatel, Switzerland
Activity: Talks and presentations › Conference presentations

**Chemical Vapour Deposition: CVD of Tantalum**
Period: 2013
James Atwoki Mugabi (Other)
Department of Energy Conversion and Storage
Proton conductors

**Description**
Part of the course - Ceramic Science and Engineering (1st lecture in spring 2013 and 2nd lecture in spring 2014)

**Related event**

Ceramic Science and Engineering
01/02/2013 → …
Denmark
**Delft Days on Magnetocalorics (2013)**
Period: 2013
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Poster presentation on the preparation of magnetocaloric perovskite.

**Related event**

**Elchemea Analytical: Software til impedans-analyse**
Period: 2013
Søren Koch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Open source software offentliggjort under GPL
Head: Søren Kock
Links:
http://www.elchemea.com

**Light trapping with plasmonic oligomers and photonic crystals to enhance the performance of organic solar cells devices**
Period: 2013 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**Complex nanophotonics**
27/08/2013 → 31/08/2013
London, United Kingdom

**Plasmonic Oligomers studies to Enhance the Performance of Organic Solar Cells devices**
Period: 2013 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**Plasmonica 2013**
01/07/2013 → 03/07/2013
Milano, Italy
Topical meeting on "Dispersion and interface chemistry" in the Danish Ceramic Society
Period: 18 Dec 2013
Michela Della Negra (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Stability studies on ceramic suspensions using complementary analysis techniques.

Topical meeting on "Dispersion and interface chemistry" in the Danish Ceramic Society.

Related event
Topical meeting on "Dispersion and interface chemistry" in the Danish Ceramic Society
18/12/2013 → …
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

Microstructure characterisation of solid oxide electrolysis cells operated at high current density
Period: 6 Dec 2013
Jacob R. Bowen (Invited speaker)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
High temperature solid oxide cells can be operated either as fuel cells or electrolysis cells for efficient power generation or production of hydrogen from steam or synthesis gas (H2 + CO) from steam and CO2 respectively. When operated under harsh conditions, they often exhibit microstructural degradation of cell components in relation to the loss of electrochemical performance specific to the mode of operation. Thus descriptive microstructure characterization methods are required in combination with electrochemical characterization methods to decipher degradation mechanisms. In the present work, microstructure evolution of the Ni-yttria stabilized zirconia (YSZ) is followed as a function of galvanostatic steam electrolysis testing at current densities between -0.5 and -1.0 A cm-2 for periods of up to 750 hours at 800 °C. The volume fraction and size of the percolating Ni particles was statistically quantified using the mean linear intercept method as a function of current density and correlated to increases in serial resistance.

The above structural changes are then compared in terms of electrode degradation observed during the co-electrolysis of steam and CO2 at current densities up to -1.5 A cm-2. In this study, the formation of ZrO2 based nano particles at the Ni-pore interface is responsible for the loss of Ni-YSZ particle contact and thus loss of triple phase boundary. Formation of similar nano particles at Ni internal grain boundaries is also thought to be responsible for loss of Ni percolation.

Related event
Thermec 2013 - International Conference on Processing & Manufacturing of Advanced Materials: Processing, Fabrication, Properties, Application
02/12/2013 → 06/12/2013
Las Vegas, United States
Activity: Talks and presentations › Conference presentations

Combined computational and experimental study of the role of CO2 poisoning on the electronic conduction and overpotentials in Li-air batteries
Period: 4 Dec 2013 → 5 Dec 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Nordisk Batterikonferens 2013 (NORDBATT)
04/12/2013 → 05/12/2013
Uppsala, Sweden
Electrospin our Energy Devices
Period: 3 Dec 2013
Wenjing (Angela) Zhang (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Invitation letter for Dr W Zhang

Related event

Electrospin Our Energy Devices
03/12/2013 → …
Adelaide, Australia
Activity: Talks and presentations › Conference presentations

Shaping our Energy Future with Electrospinning
Period: 2 Dec 2013
Wenjing (Angela) Zhang (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Invited speaker for Research Seminar in School of Chemical Engineering at The University of Adelaide.
Documents:
Seminar Abstract_20131202

Related event

School of Chemical Engineering Research Seminar
02/12/2013 → …
Adelaide, Australia
Activity: Talks and presentations › Conference presentations

the 10th International Symposium on Novel Carbon Resource Sciences
Period: 2 Dec 2013
Ngo Van Nong (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

2013 MRS Fall Meeting & Exhibit
Period: 1 Dec 2013 → 6 Dec 2013
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Documents:
MRS_Abstract

Related event
2013 MRS Fall Meeting & Exhibit  
01/12/2013 → 06/12/2013  
Boston, MA, United States  
Activity: Attending an event › Participating in or organising a conference

Design of Experiment  
Period: 26 Nov 2013 → 27 Nov 2013  
Francesca Teocoli (Participant)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Description  
Short Course: Design of Experiments. Instructors: Jakob Christensen, Umetric AB, Umeå, Sweden.  
Participation to the short course on "Design of Experiments".

Related event  
Design of Experiment  
26/11/2013 → 27/11/2013  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

3-Dimensional Nanofiber Electrodes for Solid Oxide Fuel Cells and Proton Exchange Membrane Fuel Cells  
Period: 25 Nov 2013  
Wenjing (Angela) Zhang (Lecturer)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Related event  
3-Dimensional Nanofiber Electrodes for Solid Oxide Fuel Cells and Proton Exchange Membrane Fuel Cells  
25/11/2013 → …  
Melbourne, Australia  
Activity: Talks and presentations › Conference presentations

Sustainable Fuels from Renewable Energies  
Period: 20 Nov 2013  
Mogens Bjerg Mogensen (Invited speaker)  
Department of Energy Conversion and Storage  
Fundamental Electrochemistry  
Description  
Electrolysis for conversion of H2O and CO2 into green fuels.  
Related event  
Sustainable Fuels from Renewable Energies: IASS Brainstorming Workshop  
19/11/2013 → 20/11/2013  
Potsdam, Germany  
Activity: Talks and presentations › Conference presentations

Electrochemical Energy Storage - Batteries  
Period: 14 Nov 2013  
Tejs Vegge (Invited speaker)  
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

DTU International Energy Report 2013 Symposium
14/11/2013 → …
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

ENHANCED MASS DIFFUSION PHENOMENA IN HIGHLY DEFECTIVE DOPED CERIA: LIMITS AND APPLICATIONS:
Ionic and Electronic Conductors and Applications to Solid Oxide Fuel Cells and Membrane Technology
Period: 13 Nov 2013
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
ICE2013-VIES_GDC enhanced
Links:
http://www.ice2013.net/conference-invited-speakers.php

Related event

6th International Conference on Electroceramics
09/11/2013 → 13/11/2013
João Pessoa, Brazil
Activity: Talks and presentations › Conference presentations

DTU Energy Conversion PhD symposium 2013
Period: 8 Nov 2013
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
High-temperature thermoelectric oxide modules for effective power generation from waste heat.
Links:
http://www.ecs.dtu.dk/Kalender/2013/11/PhD-symposium

Related event

DTU Energy Conversion PhD symposium 2013
08/11/2013 → 08/11/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Første symposium hos Institut for Energikonvertering- og lagring
Period: 8 Nov 2013
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Physics
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Første symposium hos Institut for Energikonvertering- og lagring
08/11/2013 → 08/11/2013
Period: 3 Nov 2013 → 6 Nov 2013
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Plenary talk

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Delft Days on Magnetocalorics (2013)
Lars von Moos (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Participant and poster presenter

Documents:
Lars_von_Moos_PosterDDMC13

Related event
Delft Days on Magnetocalorics (2013)
28/10/2013 → 29/10/2013
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

Calculational and experimental study of the role of CO2 poisoning on the electronic conduction and overpotentials in Li-air batteries
Tejs Vegge (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
224th Electrochemical Society Meeting
27/10/2013 → 01/11/2013
San Francisco, CA, United States
Activity: Talks and presentations › Conference presentations

Design and optimisation of permanent magnet systems for magnetic refrigeration
Period: 25 Oct 2013
Christian Bahl (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials
Related event

Applied Magnetic Materials
24/10/2013 → 25/10/2013
Pori, Finland
Activity: Talks and presentations › Conference presentations

13th International Symposium on Solid Oxide Fuel Cells (SOFC-XIII)
Anne Hauch (Participant)
Applied Electrochemistry
Department of Energy Conversion and Storage

Description
Participation in and oral presentation at the 13th International Symposium on Solid Oxide Fuel cells (SOFC-XIII)

Sulfur Poisoning of Ni/stabilized-zirconia Anodes – Effect on Long-Term Durability

Related event

13th International Symposium on Solid Oxide Fuel Cells (SOFC-XIII)
06/10/2013 → 11/10/2013
Okinawa, Japan
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

The Danish Energy Agreement and Solid Oxide Cells
Period: 6 Oct 2013
Anke Hagen (Lecturer)
Applied Electrochemistry

Related event

Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells)
06/10/2013 → …
Okinawa, Japan
Activity: Talks and presentations › Conference presentations

Smart Energy Conversion and Storage Conference
Period: 2 Oct 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Current Density - Overvoltage Relations for Solid Oxide Electrodes.

Invited Talk at "Smart Energy Conversion and Storage Conference".

Related event

Smart Energy Conversion and Storage Conference: IV Polish Forum
01/10/2013 → 04/10/2013
Krynica, Poland
Activity: Talks and presentations › Conference presentations

Talk on magnetocaloric research
Period: 30 Sep 2013
Lars von Moos (Speaker)
Department of Energy Conversion and Storage

Electrofunctional materials

**Description**
North Carolina State University.

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Computational screening of mixed metal halide ammines**
Period: 17 Sep 2013
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Center for Atomic-scale Materials Design

**Related event**
E-MRS 2013 Fall Meeting. Symposium C
16/09/2013 → 20/09/2013
Warsaw, Poland
Activity: Talks and presentations › Conference presentations

**From magnetocaloric materials to magnetic refrigeration devices**
Period: 10 Sep 2013
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Related event**
Donostia International Conference on Nanoscaled Magnetism and Applications
09/09/2013 → 13/12/2013
San Sebastian, Spain
Activity: Talks and presentations › Conference presentations

**Electrochemical reduction of CO2 and H2O into fuels: Cell types and kinetic barriers**
Period: 9 Sep 2013
Mogens Bjerg Mogensen (Keynote speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

**Related event**
246th American Chemical Society National Meeting : Symposium on "Electrocatalysis of Energy Generation and Storage"
08/09/2013 → 12/09/2013
Indianapolis, United States
Activity: Talks and presentations › Conference presentations

**Functional dependent errors in DFT calculations for Li-air batteries**
Period: 9 Sep 2013
Rune Christensen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Center for Atomic-scale Materials Design
Department of Physics

Description
Presentation of key conclusions from Masters thesis.

Related event
2nd ReLiable Li-Air Workshop
09/09/2013 → 10/09/2013
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Materials Predictors and Genetic Algorithms for Design of Nanoparticle Activity and Stability
Period: 3 Sep 2013 → 7 Sep 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
International Conference on Computational Modelling of Nanostructured materials, ICCMNM 2013
03/09/2013 → 07/09/2013
Frankfurt am Main, Germany
Activity: Talks and presentations › Conference presentations

1st International PhD Summer School
Period: 28 Aug 2013
Jacob R. Bowen (Lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Microscopy methods for advanced ceramics
Course lecturer

Related event
1st International PhD Summer School: Optimized Processing of Multi-material Architectures for Functional Ceramics
26/08/2013 → 31/08/2013
Roskilde, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

1st Workshop in Prof. John Irvine's EPSRC Platform project
Period: 28 Aug 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Title: Reversible oxide cells: Visions, limitations and possibilities.
Participated as member of the advisory committee of Prof. John Irvine's (St. Andrews University, Scotland) EPSRC Platform project, and gave an invited talk.

Related event
1st Workshop in Prof. John Irvine's EPSRC Platform project  
27/08/2013 → 28/08/2013  
Aviemore, Scotland, United Kingdom  
Activity: Talks and presentations › Conference presentations

1st International PhD Summer School  
Period: 26 Aug 2013 → 31 Aug 2013  
Francesca Teocoli (Participant)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Related event  
1st International PhD Summer School: Optimized Processing of Multi-material Architectures for Functional Ceramics  
26/08/2013 → 31/08/2013  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

1st PhD summer school  
Period: 26 Aug 2013 → 30 Aug 2013  
Thanh Hung Le (Participant)  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Documents:  
PhD_summer_school_Thanh_Hung_Le_Abstract  
Links:  
http://indico.conferences.dtu.dk/conferenceDisplay.py?ovw=True&confid=130  
Related event  
1st PhD summer school  
26/08/2013 → 30/08/2013  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

The challenges in going from magnetocaloric materials to magnetic refrigeration devices  
Period: 29 Jul 2013  
Christian Bahl (Invited speaker)  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Related event  
SPP 1599 Convention  
29/07/2013 → 01/08/2013  
Lichtenfels, Germany  
Activity: Talks and presentations › Conference presentations

Eurotech participants meeting  
Period: 17 Jul 2013  
Michael Corazza (Speaker)  
Department of Energy Conversion and Storage  
Functional organic materials  
Description  
Eurotech participants meeting
Related event

Eurotech participants meeting
17/07/2013 → 18/07/2013
Munich, Germany
Activity: Talks and presentations › Conference presentations

Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop
Period: 11 Jul 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
SOFC Funding Assessment Committee Contribution A presentation about possible strategies based on my long experience inside the area of SOFC R&D.

Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop. A workshop on solid oxide fuel cell R&D strategies.

Related event

Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop
11/07/2013 → 12/07/2013
Arlington, United States
Activity: Talks and presentations › Conference presentations

32nd International Conference on Thermoelectrics
Period: 30 Jun 2013 → 4 Jul 2013
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Links:
http://ict2013.its.org/

Related event

32nd International Conference on Thermoelectrics
30/06/2012 → 04/07/2013
Kobe, Japan
Activity: Attending an event › Participating in or organising a conference

Materials for energy storage – screening and evolution
Period: 25 Jun 2013 → 30 Jun 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

SUNCAT Summer School
25/06/2013 → 30/06/2013
Stanford, United States
Activity: Talks and presentations › Conference presentations

Computational screening and design of energy materials – navigating vast phase spaces
Period: 24 Jun 2013 → 28 Jun 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Solar Fuels Summer School
24/06/2013 → 28/06/2013
Reykjavik, Iceland
Activity: Talks and presentations › Conference presentations

Arthur S. Nowick Memorial Symposium
Period: 7 Jun 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Invited presentation: Volume of Oxide Vacancies in Fluorite and Perovskite Structured Oxides.
Invited participant in Arthur S. Nowick Memorial Symposium.

Related event

Arthur S. Nowick Memorial Symposium
07/06/2013 → …
Kyoto, Japan
Activity: Talks and presentations › Conference presentations

Reversible solid oxide cells: limitations and possibilities
Period: 4 Jun 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Invited presentation at and participation in 19th International Conference on Solid State Ionics.
Documents:
\iri-filab\home\momo\My Documents\Conferences and meetings\SSI-19\REVERSIBLE SOLID OXIDE CELLS LIMITATIONS AND POSSIBILITIES\SSI-19_Abstract_Invited_Mogens

Related event

19th International Conference on Solid State Ionics
02/06/2013 → 07/06/2013
Kyoto, Japan
Activity: Talks and presentations › Conference presentations

10th Pacific Rim Conference on Ceramic and Glass Technology
Period: 2 Jun 2013 → 7 Jun 2013
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Poster presentation.
Documents:
Abstract_PACRIM10_Teocoli_Francesca
Related event

10th Pacific Rim Conference on Ceramic and Glass Technology
02/06/2013 → 07/06/2013
San Diego, CA, United States
Activity: Attending an event › Participating in or organising a conference

Sintering of Ceramics
Period: 1 Jun 2013 → 2 Jun 2013
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Short Course: Sintering of Ceramics. Instructors: Mohamed N. Rahaman, Missouri University of Science and Technology.

Participation to the short course on "Sintering of Ceramics".

Related event

Sintering of Ceramics
01/06/2013 → 02/06/2013
San Diego - California, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Inorganic Chemistry (Journal)
Period: May 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Inorganic Chemistry

Related journal

Inorganic Chemistry
0020-1669
Central database
Activity: Research › Peer review of manuscripts

Sustainable fuels from renewable energy
Period: 22 May 2013
Mogens Bjorg Mogensen (Lecturer)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Spring School: Smart energy Solutions in Urban Environment.

Related event

Spring School: Smart energy Solutions in Urban Environment
21/05/2013 → 25/05/2013
Pra Catinat, Italy
Activity: Talks and presentations › Conference presentations
Seminar Activity in Politecnico di Torino
Period: 21 May 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Title of presentation: Sustainable fuels from renewable energy.
Seminar Activity in Politecnico di Torino.

Related event
Seminar Activity in Politecnico di Torino
21/05/2013 → …
Torino, Italy
Activity: Talks and presentations › Conference presentations

9th International Symposium on Hysteresis Modelling and Micromagnetics
Period: 13 May 2013 → 15 May 2013
Lars von Moos (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
9th International Symposium on Hysteresis Modelling and Micromagnetics
13/05/2013 → 15/05/2013
Taormina, Italy
Activity: Talks and presentations › Conference presentations

Journal of Alloys and Compounds (Journal)
Period: Apr 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of Alloys and Compounds

Related journal
Journal of Alloys and Compounds
0925-8388
Central database
Activity: Research › Peer review of manuscripts

Materials Research Bulletin (Journal)
Period: Apr 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Related journal

Materials Research Bulletin

Central database
Activity: Research › Peer review of manuscripts

International Energy Agency
Period: 21 Apr 2013 → 25 Apr 2013
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
NH3 Storage in Mixed Salt – MH-Air Cell

Related event

International Energy Agency: Kickoff Meeting of Task 32 "Hydrogen-based energy storage"
21/04/2013 → 25/04/2013
Heraklion - Crete, Greece
Activity: Talks and presentations › Conference presentations

The 5th Fundamentals and Developments of Fuel Cells Conference 2013
Period: 17 Apr 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Operation temperature, materials and reversibility of fuel cells - electrolyser cells.

Related event

The 5th Fundamentals and Developments of Fuel Cells Conference 2013
16/04/2013 → 18/04/2013
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations

Identifying Ways to Improve the Efficiency of Magnetocaloric Devices
Period: 15 Apr 2013 → 19 Apr 2013
Christian Bahl (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Joint Workshop (DTU and Federal University of Santa Catarina, Florianopolis, Brazil)
"Identifying Ways to Improve the Efficiency of Magnetocaloric Devices"
Funded by Danish Agency for Science, Technology and Innovation and to the CNPq, Brazil

Related event

Identifying Ways to Improve the Efficiency of Magnetocaloric Devices
15/04/2013 → 19/04/2013
Florianopolis, Brazil
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Identifying Ways to Increase the Efficiency of Magnetocaloric Devices**
Period: 15 Apr 2013 → 19 Apr 2013
Lars von Moos (Speaker)
Risø National Laboratory for Sustainable Energy
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Identifying ways to increase the efficiency of magnetocaloric devices

**Related event**

**Identifying Ways to Increase the Efficiency of Magnetocaloric Devices**
15/04/2013 → 19/04/2013
Florianopolis, Brazil
Activity: Talks and presentations › Conference presentations

**Using biofuels for SOFC**
Period: 13 Apr 2013
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related event**

**2nd International Symposium on Solid Oxide Fuel Cells for Next Generation Power Plants: SOFCs and Renewable Energy**
19/04/2013 → …
London, United Kingdom
Activity: Talks and presentations › Conference presentations

**Electrolysis and CO2-Recycling for Production of Green Fuels**
Period: 9 Apr 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

**Description**
Indlæg ved Conference

**Related event**

**Electrolysis and CO2-Recycling for Production of Green Fuels**
09/04/2013 → 11/04/2013
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

**Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels**
Period: 9 Apr 2013 → 11 Apr 2013
Mogens Bjerg Mogensen (Organizer)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

**Description**
Co-chairman together with Prof. Klaus S. Lackner, Columbia University, NY, USA.

Co-chair and organizer of the workshop: Electrolysis and CO2-Recycling for Production of Green Fuels
Related event

**Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels**

*Period: 9 Apr 2013*

Mogens Bjerg Mogensen (Speaker)

Fundamental Electrochemistry

Description

**Perspectives in Electrolysis and CO2-Recycling.**

Introductory talk "Perspectives in Electrolysis and CO2-Recycling" to the Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels.

Related event

**Computational screening of mixed metal halide ammines**

*Period: 8 Apr 2013*

Peter Bjerre Jensen (Lecturer)

Department of Energy Conversion and Storage

Theoretical Atomic-scale Physics

Atomic scale modelling and materials

Related event

**245th ACS National Meeting & Exposition**

*Period: 20 Mar 2013*

Søren Linderoth (Lecturer)

Department of Energy Conversion and Storage

Related event

**Collaboration between DTU and Topsoe Fuel Call**

*Period: 9 Mar 2013*

Søren Linderoth (Speaker)

Department of Energy Conversion and Storage

Related event

**Open Inspiration : Denmark - the green test land of oppotunity**

*Period: 20 Mar 2013*

Kgs. Lyngby, Denmark

Activity: Talks and presentations › Conference presentations

Related event

**Renewable Energy Technologies: Possible Collaboration Between Denmark and Japan**

*Period: 9 Mar 2013*

Søren Linderoth (Speaker)

Department of Energy Conversion and Storage
Related event

Pugwash: Remembering Fukushima
09/03/2013 → …
København, Denmark
Activity: Talks and presentations › Conference presentations

Electronic Materials Letters (Journal)
Period: Feb 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related journal

Electronic Materials Letters
1738-8090
Scopus rating (2016): CiteScore 1.58 SJR 0.519 SNIP 0.872, Web of Science (2017): Indexed Yes
Local database
Activity: Research › Peer review of manuscripts

Department of Energy Conversion and Storage
Period: 26 Feb 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Related event

Korean-Danish Green Technology Workshop
25/02/2013 → 27/02/2013
Seoul, Korea, Republic of
Activity: Talks and presentations › Conference presentations

3rd Magnetism National Conference
Period: 20 Feb 2013 → 22 Feb 2013
Lars von Moos (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Participation in conference
Documents:
Poster_Magnet2013

Related event

3rd Magnetism National Conference
20/02/2013 → 22/02/2013
Naples, Italy
Activity: Attending an event › Participating in or organising a conference

Nanostructured materials for solid-state hydrogen storage – WG4: Computational modeling
Period: 25 Jan 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
PALSfit; website: palsfit.dk: A computer code for analysing positron annihilation lifetime spectra.

Description
PALSfit is a computer program for analysing spectra that are measured by positron annihilation lifetime spectroscopy (PALS). PALSfit is based on the well tested PATFIT program, which has been used extensively by the positron annihilation community. Taking advantage of the windows interface, a number of user friendly facilities have been incorporated, in particular graphics displays.

Links:
http://palsfit.dk
Department of Micro- and Nanotechnology
Molecular Windows
Degree of recognition: International

Related external organisation
American Physical Society
United States
Activity: Membership › Membership of research networks or expert groups

Applied Physics Letters (Journal)
Period: 2012 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows

Description
I work quite regularly as a reviewer for Applied Physics Letters in the topic of nanomagnetism and spintronics from 2012

Related journal
Applied Physics Letters
0003-6951
Central database
Activity: Research › Peer review of manuscripts

PhD thesis Alfred Samson: Censor
Period: 2012
Anke Hagen (External examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Activity: Examinations and supervision › External examination

Self assembled dimers of metallic nano-particles for enhanced light harvesting in organic solar cells
Period: 2012 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event
5th Mediterranean Conference on NanoPhotonics
05/11/2012 → 06/11/2012
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

Self assembled dimers of metallic nano-particles for enhanced light harvesting in organic solar cells
Period: 2012 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

*Conferencia Española de Nanofotonica 2012*

01/10/2012 → 04/10/2012
Sevilla, Spain

Activity: Talks and presentations › Conference presentations

**Strategy Group (External organisation)**

Period: 2012 → 2015
Anke Hagen (Participant)

Department of Energy Conversion and Storage

Applied Electrochemistry

**Description**

Under Partnership for Hydrogen and Fuel Cells

**Related external organisation**

**Strategy Group**

Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar

**Ergebnisse aus Langzeittests von Einzelzellen**

Period: Dec 2012
Anke Hagen (Lecturer)

Department of Energy Conversion and Storage

Applied Electrochemistry

**Related event**

*2nd SOFC Workshop „Reproduzierbares Testen von SOFC Einzelzellen - aktuelle Entwicklungen in Standardisierung und Charakterisierung“*

17/12/2012 → 18/12/2012
Barleben, Germany

Activity: Talks and presentations › Conference presentations

**Design, Modeling and Optimization of Thermoelectrical Power Generation Devices**

Period: 10 Dec 2012
Nini Pryds (External examiner)

Department of Energy Conversion and Storage

Electrofunctional materials

**Description**

PHD Examiner

Activity: Examinations and supervision › External examination

**Nordic Conference on Ceramic and Glass Technology**

Period: 6 Dec 2012 → 7 Dec 2012
Francesca Teocoli (Participant)

Department of Energy Conversion and Storage

Ceramic Engineering & Science

**Description**

Shape distortion and thermo-mechanical properties of SOFC components from green tape to sintered body

Documents:
Abstract_Nordic_Conference_Teocoli.pdf

Related event

**Nordic Conference on Ceramic and Glass Technology**
06/12/2012 → 07/12/2012
Roskilde, Denmark
Activity: Attending an event › Participating in or organising a conference

**Computational Screening of Mixed Metal Halide Ammines**
Period: 4 Dec 2012
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Department of Physics

Related event

**1st European Early Stage Researchers’ Conference on Hydrogen Storage**
03/12/2012 → 05/12/2012
Belgrade, Serbia
Activity: Talks and presentations › Conference presentations

**6th International Workshop on Advanced Materials Science and Nanotechnology**
Period: Nov 2012
Ngo Van Nong (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Nanostructured Thermoelectric Oxide Materials and Modules for Effective Power Generation from Waste Heat

Related event

**6th International Workshop on Advanced Materials Science and Nanotechnology**
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

**Degradation of state-of-the-art SOFC in hydrogen and carbon containing fuels**
Period: Nov 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

**Workshop on Sulfur Poisoning of Solid Oxide Cells, Risø Campus**
19/11/2012 → …
Risø, Denmark
Activity: Talks and presentations › Conference presentations

**2012 MRS Fall Meeting & Exhibit**
Nini Pryds (Organizer)
Electrofunctional materials

**Description**
Oxide Thin Films for Renewable Energy Applications

**Related event**

*2012 MRS Fall Meeting & Exhibit*
25/11/2012 → 30/11/2012
Boston, MA, United States
Activity: Attending an event › Participating in or organising a conference

**Electrolysis and biomass hand-in-hand**
Period: 15 Nov 2012
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage
Management

**Related event**

*Conference on Energy Security: Outlook & Perspectives in the Baltic Sea Region*
15/11/2012 → 16/11/2012
Vilnius, Lithuania
Activity: Talks and presentations › Conference presentations

**Oxides in Environment-friendly Technologies**
Period: 3 Nov 2012
Nini Pryds (Invited speaker)
Electrofunctional materials
Department of Energy Conversion and Storage

**Description**
Invited speaker at our G-COE International Symposium, Japan
http://ncrs.cm.kyushu-u.ac.jp/ncrs2/home.html
Oxides in Environment-friendly Technologies

**Related external organisation**

*Unknown external organisation*
Activity: Talks and presentations › Conference presentations

**Final SERC Technical-Scientific Meeting**
Period: 1 Nov 2012
Peter Blennow Tullmar (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
Presented a summary of the results obtained within SERC on new materials for solid oxide cells
New materials for solid oxide cells - nanostructured electrocatalysts by infiltration and/or exsolution

**Related event**

*Final SERC Technical-Scientific Meeting*
01/11/2012 → …
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

**Ceramics International (Journal)**
Period: Oct 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Ceramics International

**Related journal**
Ceramics International
0272-8842
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 2.88 SJR 0.853 SNIP 1.304, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

**6th International Workshop on Advanced Materials Science and Nanotechnology**
Thanh Hung Le (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Geometry optimization on high temperature oxide thermoelectric power generation
Oral presentation

**Related event**
6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

6th International Workshop on Advanced Materials Science and Nanotechnology
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
High-Temperature segmented thermoelectric oxide module using p-type $\text{Ca}_3\text{Co}_4\text{O}_9$ and n-type $\text{ZnAlO/CaMn}_{0.95}\text{Nb}_{0.05}\text{O}$ 3 legs

**Documents:**
Abstract

**Related event**
6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations
THE INFLUENCE OF BORON ADDITION ON STRUCTURAL, MAGNETIC AND THERMOELECTRIC PROPERTIES OF Ni$_2$Mn$_{1.52}$Sb$_{0.48}$B$_x$
Electrofunctional materials

Related event

**Applied Magnetic Materials**
24/10/2013 → 25/10/2013
Pori, Finland
Activity: Talks and presentations › Conference presentations

**International Symposium on Metal-Hydrogen Systems - Fundamentals and Applications** -
Didier Blanchard (Participant)

Department of Energy Conversion and Storage

**Description**
Two Posters presentations - QENS in Ca and Mg Borohydrides - Ammonia Storage in Metal Salts

Related event

**International Symposium on Metal-Hydrogen Systems - Fundamentals and Applications** -
21/10/2012 → 26/10/2012
Kyoto, Japan
Activity: Attending an event › Participating in or organising a conference

**Metal Borohydrides for Hydrogen Storage: A Review**
Period: 21 Oct 2012
Didier Blanchard (Invited speaker)

Department of Energy Conversion and Storage

**Description**
Atomic scale modelling and materials

Related event

**BiT's 2nd New Energy Forum - 2012: Hydrogen energy**
19/10/2012 → 21/10/2012
Guangzhou, China
Activity: Talks and presentations › Conference presentations

**Department of Energy Conversion and Storage**
Period: 17 Oct 2012
Søren Linderoth (Lecturer)

Department of Energy Conversion and Storage

**Description**
Oplæg ved SK Innovation Global Technology, Daejeon, Korea

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Solid oxide electrochemical cells – energy converters, gas separators, gas sensors**
Period: 14 Oct 2012
Mogens Bjerg Mogensen (Lecturer)

Fundamental Electrochemistry

Department of Energy Conversion and Storage
Related event

INANO Autumn School 2012
12/10/2012 → 15/10/2012
Grenå, Denmark
Activity: Talks and presentations › Conference presentations

SERC Workshop
Period: 8 Oct 2012
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Computational investigations of the electronic transport in lithium-air battery materials
Tejs Vegge (Speaker)
Department of Energy Conversion and Storage

Pacific Rim Meeting on Electrochemical and Solid-State Science: 222nd Meeting of ECS — The Electrochemical Society and 2012 Fall Meeting of The Electrochemical Society of Japan
07/10/2012 → 12/10/2012
Honolulu, United States
Activity: Talks and presentations › Conference presentations

Istituto Nazionale di Ricerca Metrologica
Period: 1 Oct 2012 → 17 Dec 2012
Lars von Moos (Visiting researcher)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Research stay: Collaboration with research group
Activity: Visiting an external institution › Visiting another research institution

Journal of Electronic Materials (Journal)
Period: Sep 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of Electronic Materials

Related journal
Journal of Electronic Materials
Pure and Applied Chemistry (Journal)
Period: Sep 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Pure and Applied Chemistry

Related journal
Pure and Applied Chemistry
0033-4545
Central database
Activity: Research › Peer review of manuscripts

Solid State Electrochemistry Applied to Solid Oxide Fuel and Electrolysis Cells
Period: Sep 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Electrochemistry 2012
17/09/2012 → 23/09/2012
München, Germany
Activity: Talks and presentations › Conference presentations

Alkaline Electrolysis Cells: Materials, Properties and Challenges
Period: 25 Sep 2012
Mogens Bjerg Mogensen (Lecturer)
Fundamental Electrochemistry
Department of Energy Conversion and Storage
Department of Physics

Description
Lecture at 2nd Joint European Summer School on Fuel Cells and Hydrogen Technology.

Related event
2nd Joint European Summer School on Fuel Cell and Hydrogen Technology
17/09/2012 → 28/09/2012
Heraklion, Greece
Activity: Talks and presentations › Conference presentations

History of Thermodynamics of Electrolysis
Period: 25 Sep 2012
Mogens Bjerg Mogensen (Lecturer)
Fundamental Electrochemistry
Department of Energy Conversion and Storage
Department of Physics

Description
Lecture at 2nd Joint European Summer School on Fuel Cells and Hydrogen Technology

Related event
2nd Joint European Summer School on Fuel Cell and Hydrogen Technology
17/09/2012 → 28/09/2012
Heraklion, Greece
Activity: Talks and presentations › Conference presentations

5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 18 Sep 2012
Christian Bahl (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Invited speaker
Development and Experimental Results from a 1 kW Prototype AMR

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 18 Sep 2012
Kurt Engelbrecht (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Gave presentation titled "Material Properties and Modeling Characteristics for MnFePAs Materials for Application in Magnetic Refrigeration"

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 18 Sep 2012
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Development and Experimental Results from a 1kW Prototype AMR
Period: 18 Sep 2012
Christian Bahl (Invited speaker)
Electrofunctional materials

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 17 Sep 2012 → 20 Sep 2012
Lars von Moos (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Talk at Thermag 5 Conference, Grenoble Italy

**Related event**
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
17/09/2012 → 20/09/2012
Grenoble, France
Activity: Talks and presentations › Conference presentations

ESS Science Symposium
Period: 17 Sep 2012 → 19 Sep 2012
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Poster presentation

**Related event**
ESS Science Symposium: Neutrons for Energy - Advanced Materials for Energy Storage
17/09/2012 → 19/09/2012
Delft, Netherlands
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

3rd CARISMA International Conference on Medium and High Temperature Proton Exchange Membrane Fuel Cells
Period: 3 Sep 2012
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

**Related event**
3rd CARISMA International Conference on Medium and High Temperature Proton Exchange Membrane Fuel Cells
03/09/2012 → 05/09/2012
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Årsmøde 2013 i Dansk Batteriselskab
Period: 1 Sep 2012 → 1 Mar 2013
Jonathan Højberg (Organizer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Medstifter af Dansk Batteriselskab og medarrangør af arrangementet

Links:
http://batteriselskab.dk/founding_meeting
**Related event**

Årsmøde 2013 i Dansk Batteriselskab  
01/03/2013 → 01/03/2013  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising a conference

**SUNCAT Center for Interface Science and Catalysis**  
Period: 1 Sep 2012 → 30 Nov 2012  
Tejs Vegge (Visiting researcher)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  
Description  
Visiting Professor: SUNCAT at SLAC National Accelerator and Department of Chemical Engineering, Stanford University  
Activity: Visiting an external institution › Visiting another research institution

**Vacuum (Journal)**  
Period: Aug 2012 → 00/00/0000  
Ngo Van Nong (Reviewer)  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Description  
Vacuum  
Related journal  
**Vacuum**  
0042-207X  
Central database  
Activity: Communication › Peer review of manuscripts

**Computational Design of Materials for Energy Storage**  
Period: 11 Aug 2012 → 17 Aug 2012  
Tejs Vegge (Invited speaker)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  
Related event  
**CAMD Summer School in Electronic Structure Theory and Materials Design**  
11/08/2012 → 17/08/2012  
Lyngby, Denmark  
Activity: Talks and presentations › Conference presentations

**Reversible Lithium-Air Batteries**  
Period: 10 Aug 2012  
Tejs Vegge (Lecturer)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  
Related event
In situ XRPD studies of Li intercalation in graphite in working Li-ion batteries: Session: MS13 - Energy related materials
Rune E. Johnsen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

27th Meeting of the European Crystallographic Association
06/08/2012 → 11/08/2012
Bergen, Norway
Activity: Talks and presentations › Conference presentations

A Materials Science Perspective on the Mechanics of Sintering
Period: 20 Jul 2012
Rasmus Bjørk (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Presented at: CEA Cadarache, France

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

12th International Conference on Inorganic Membrane
Period: 13 Jul 2012
Kurt Engelbrecht (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Mechanical analysis of tubular oxygen membranes for robust membrane modules

Related event

31st International & 10th European Conference on Thermoelectrics
Period: 11 Jul 2012
Li Han (Speaker)
Department of Energy Conversion and Storage

Description
Presentation of ‘The Influence of Spark Plasma Sintering Temperature on the Thermoelectric Properties of Al, Ga dually-doped ZnO’
31st International & 10th European Conference on Thermoelectrics
Period: 9 Jul 2012
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Oral presentation

Related event

Plasma Sheath Lenses - Principles and applications
Period: 2 Jul 2012 → 6 Jul 2012
Eugen Stamate (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
award invited lecture

Related event

European Fuel Cell Forum 2012
Period: 30 Jun 2012 → 3 Jul 2012
Anne Hauch (Participant)
Applied Electrochemistry
Department of Energy Conversion and Storage

Description
Deltager samt poster bidrag

Multilayer Tape Cast SOFC - Effect of Anode Sintering Temperature
Documents:
EFCF_poster_cbir_2012-06-22_hauc_edit_FINAL

Related event
European Fuel Cell Forum 2012  
Peter Blennow Tullmar (Speaker)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Description  
Poster presentation at the conference: Infiltrated SrTiO$_3$:FeCr-based anodes for metal-supported SOFC  
Related event  
European Fuel Cell Forum 2012  
27/06/2012 → 29/06/2012  
Luzern, Switzerland  
Activity: Talks and presentations › Conference presentations

Rotational and translational diffusion in materials for energy storage from QENS and DFT calculations  
Tejs Vegge (Invited speaker)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  
Related event  
2nd Annual Niels Bohr International Academy Workshop on Neutron Science: Bridging Elastic and Inelastic Scattering by means of Computational Studies and Analysis  
25/06/2012 → 29/06/2012  
Copenhagen, Denmark  
Activity: Talks and presentations › Conference presentations

Computational techniques for efficient design of nanoparticles and complex materials for energy storage  
Period: 13 Jun 2012 → 18 Jun 2012  
Tejs Vegge (Lecturer)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  
Related event  
International Conference on Materials for Hydrogen Storage – Future and Perspectives  
13/06/2012 → 18/06/2012  
Hurtigruten, Norway  
Activity: Talks and presentations › Conference presentations

Development of SOEC Cells and Stacks: Highlights, Challenges and future Perspectives  
Period: 5 Jun 2012  
Wolff-Ragnar Kiebach (Keynote speaker)  
Department of Energy Conversion and Storage  
Mixed Conductors  
Related event  
World Hydrogen Energy Conference 2012  
03/06/2012 → 07/06/2012  
Toronto, Canada  
Activity: Talks and presentations › Conference presentations
Mundtligt oplæg ved besøg hos Samsung Advanced Institute of Technology (SAIT, Suwan, Korea

SOFC Durability under Realistic Operation
Period: May 2012
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
Period: May 2012
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
10/05/2012 → 11/05/2012
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

42nd Danish Crystallographic Meeting and 5th DanScatt Meeting
Period: 31 May 2012 → 1 Jun 2012
Rune E. Johnsen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Poster presentation: "In situ synchrotron X-ray diffraction studies of large and small lithium batteries (from 10Ah to 0.1 mAh)"

**Related event**

**42nd Danish Crystallographic Meeting and 5th DanScatt Meeting**
31/05/2012 → 01/06/2012
Odense, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**European Materials Research Society 2012**
Period: 30 May 2012
Li Han (Participant)
Department of Energy Conversion and Storage

**Description**
Presentation of 'the influence of including α- or γ-Al2O3 phases in Al-doped ZnO on the Thermoelectric Properties'

**Related event**

**European Materials Research Society 2012: Symposium D, Unconventional Thermoelectrics: From new materials to energy conversion devices**
27/05/2012 → 31/05/2012
Strasbourg, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Oxford Instruments EBSD Symposium**
Period: 24 May 2012
Jacob R. Bowen (Speaker)
Department of Energy Conversion and Storage

**Imaging and Structural Analysis**

**Description**
FIB Damage and Polishing in 3DEBSD of ceramic materials

**Oxford Instruments EBSD user group meeting**
Talk Title: FIB Damage and Polishing in 3DEBSD of ceramic materials
Documents:
FIB Damaging and Polishing in 3DEBSD of ceramic materials

**Related event**

**Oxford Instruments EBSD Symposium**
23/05/2012 → 24/05/2012
Weisbaden, Germany
Activity: Talks and presentations › Conference presentations

**European Materials Research Society 2012**
Period: 14 May 2012
Thahn Hung Le (Participant)
Department of Energy Conversion and Storage

**Electrofunctional materials**

**Description**
Poster presentation
Related event

European Materials Research Society 2012: Symposium D, Unconventional Thermoelectrics: From new materials to energy conversion devices
27/05/2012 → 31/05/2012
Strasbourg, France
Activity: Attending an event › Participating in or organising a conference

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
Period: 10 May 2012 → 11 May 2012
Jacob R. Bowen (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Selected hydrogen production activities at the Institut of Technical Thermodynamics of DLR focused on the electrodes and stack design

The Institute of Technical Thermodynamics started developing various kinds of electrolysers for a large range of applications approx. in 1985. The main topics are the development of stabilized electrodes for applications with drastic load changes and high durability as well as the understanding of mechanisms and degradation effects.

Documents:
Selected hydrogen production activities at the Institute of Technical Thermodynamics of DLR focused on the electrodes and stack design

Links:
http://indico.conferences.dtu.dk/conferenceDisplay.py?confId=102 (Symposium website)

Related event

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
10/05/2012 → 11/05/2012
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Metal-supported Solid Oxide Fuel Cells: Next generation SOFCs?: Invited talk
Period: 30 Mar 2012
Peter Blennow Tullmar (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event

Lund Fuel Cell Research Network meeting
30/03/2012 → 30/03/2012
Lund, Sweden
Activity: Talks and presentations › Conference presentations

4th User Meeting at the FRM II
Period: 23 Mar 2012
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster Presentation - Hindered rotational energy barriers of BH4 - tetrahedra in beta-Mg(BH4)2 from quasielastic neutron scattering and DFT calculations

User Meeting at FRM II - Munich
**Related event**

4th User Meeting at the FRM II
23/03/2012 → ...
Munich, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Reconstructions at complex oxide Interfaces**
Period: 23 Mar 2012
Nini Pryds (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Members of the examining committee.
Activity: Examinations and supervision › External examination

**Tohoku University**
Dadi Þorsteinn Sveinbjörnsson (Visiting researcher)
Department of Energy Conversion and Storage

Description
External research stay
Activity: Visiting an external institution › Visiting another research institution

**Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103**
Peter Bjerre Jensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Department of Physics

**Related event**

Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
13/02/2012 → 15/02/2012
Roma, Italy
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Presentation of the research activities on Solid-State Hydrogen Storage at DTU -Energy Conversion and Storage.

Oral presentation

**Related event**

Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
13/02/2012 → 15/02/2012
Roma, Italy
Activity: Talks and presentations › Conference presentations
Thermoelectric Oxide Materials for Heat Recovery
Period: 9 Feb 2012
Nini Pryds (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Durability of Solid Oxide Fuel Cells and Solid Oxide Electrolysis Cells: Status and Challenges
Period: Jan 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Meeting of the SOFC Society of Japan
20/01/2012 → …
Tokyo, Japan
Activity: Talks and presentations › Conference presentations

European Fuel Cell Forum (External organisation)
Period: Jan 2012 → Jun 2012
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Member of Scientific Committee
Degree of recognition: International

Related external organisation
European Fuel Cell Forum
Obergadshalde 2, CH-6043, Luzern-Adligenswil, Switzerland
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Ph.D. defense Rahimullah Sarban: "Active control using DEAP transducers"
Period: 30 Jan 2012
Peter Sommer-Larsen (External examiner)
Department of Energy Conversion and Storage

Description
Censor: Ph.D. defense Rahimullah Sarban: "Active control using DEAP transducers"
Activity: Examinations and supervision › External examination

Studienævem DTU Energi (External organisation)
Period: 1 Jan 2012 → 31 Dec 2015
Anne Hauch (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Formand for DTU Energis studienævn
Body type: Institutstudienævn

Related external organisation

Studienævn DTU Energi
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells) (External organisation)
Period: 2011 → 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Degree of recognition: International

Related external organisation

Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells)
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

PhD Thesis Alfred Samson
Period: 2011 → Apr 2012
Anke Hagen (Internal examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Activity: Examinations and supervision › Internal examination

Thin Solid Films (Journal)
Period: 2011 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows

Description
I have regularly worked as referee for the journal of Thin Solid Films since 2011

Related journal
Thin Solid Films
0040-6090
BFI (2018): BFI-level 1, Scopus rating (2016): CiteScore 1.83 SJR 0.64 SNIP 0.897, ISI indexed (2013): ISI indexed yes, Web of Science (2017): Indexed Yes
Central database
Activity: Research › Peer review of manuscripts

2nd International Workshop on Degradation Issues of Fuel Cells
Period: Sep 2011
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related event

2nd International Workshop on Degradation Issues of Fuel Cells
Thessaloniki, Greece
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Assessing durability of SOFC stacks
Period: Sep 2011
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

2nd Workshop on Degradation Issues
05/09/2011 → 09/09/2011
Thessaloniki, Greece
Activity: Talks and presentations › Conference presentations

Journal of Alloys and Compounds (Journal)
Period: Sep 2011 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of alloys and compounds

Related journal

Journal of Alloys and Compounds
0925-8388
BFI (2018): BFI-level 2, Scopus rating (2016): CiteScore 3.05 SJR 0.961 SNIP 1.321, ISI indexed (2013): ISI indexed yes,
Web of Science (2017): Indexed yes
Central database
Activity: Research › Journal editor

Proton conductivity – mechanisms and materials
Qingfeng Li (Lecturer)
Department of Energy Conversion and Storage
Proton conductors

Related event

PROCON Summer school
16/08/2011 → 17/08/2011
Changchun, China
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Troisième Cycle Seminar in Villars
Li Han (Participant)
Department of Energy Conversion and Storage

Related event
Troisième Cycle Seminar in Villars: Synthesis and Function of Thermoelectric Materials
14/08/2011 → 18/08/2011
Villars-sur-Ollon, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Troisième Cycle Seminar in Villars
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
It is a summer school for PhD student.

Workshop on Synthesis and Function of Thermoelectric Materials

Related event

Troisième Cycle Seminar in Villars: Synthesis and Function of Thermoelectric Materials
14/08/2011 → 18/08/2011
Villars-sur-Ollon, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Durability and degradation of SOFCs – Where are we?
Period: May 2011
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells)
09/05/2011 → …
Montreal, Canada
Activity: Talks and presentations › Conference presentations

University of New South Wales
Period: 1 Mar 2011 → 31 May 2011
Jacob R. Bowen (Visiting researcher)
Fuel Cells and Solid State Chemistry Division
Microstructures and Interfaces
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Visiting Fellow

School of Materials Science and Engineering and the Electron Microscope Unit, UNSW
Links:
http://www.materials.unsw.edu.au/ (School of Materials Science and Engineering website)
Activity: Visiting an external institution › Visiting another research institution

5th International Symposium Hydrogen & Energy
Period: 23 Jan 2011 → 28 Jan 2011
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Oral Presentation: Hydrogen Rotational and Diffusional dynamics in calcium borohydride from Quasielastic Neutron Scattering and DFT.

**Related event**
5th International Symposium Hydrogen & Energy: Empa
23/01/2011 → 28/01/2011
Stoos, Switzerland
Activity: Attending an event › Participating in or organising a conference

**European Association for Storage of Energy - EASE (External organisation)**
Period: 1 Jan 2011 → 31 Dec 2017
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

**Description**
Collaboration on information and lobbying about energy storage technologies

Body type: Industry dominated private
Degree of recognition: International

**Related external organisation**
European Association for Storage of Energy - EASE
Activity: Membership › Board duties in companies, associations, or public organisations

**European Energy Research Alliance, Joint Programme on Energy Storage (External organisation)**
Period: 1 Jan 2011 → 1 Jan 2018
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

**Description**
Steering Committee
Degree of recognition: International

**Related external organisation**
European Energy Research Alliance, Joint Programme on Energy Storage
Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar

**Heavy ions doping coupled with metallic nanoincludeions: An effective way to improve the thermoelectric performance of p-type layered cobalt oxide materials: 30th International Conference on Thermoelectrics-ICT2011**
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage

**Description**
Place: Traverse City, Michigan, USA

**Related external organisation**
Unknown external organisation
Activity: Talks and presentations › Conference presentations
Recent Progress in Nanostructured Oxide TE Materials for Power Generation at High Temperatures: "Workshop on Advanced Materials Science and Nanotechnology"
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage

Description
Place: Hanoi, Vietnam

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Recent Progress in Nanostructured Thermoelectric Oxide Materials at Risø DTU: Workshop on Nanothermoelectrics
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage

Description
Place: Nya Festsalen, AF Borgen, 2011, Lund, Sweden

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Design and fabrication of broadband anti-reflection sub-wavelength periodic structure for solar cells
Period: 2010 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage

Functional organic materials

Related event

Renewable energy
27/06/2010 → 02/07/2010
Yokohama, Japan
Activity: Talks and presentations › Conference presentations

Period: 2010 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows

Description
Peer review journal

I have worked for Materials Science and Engineering B, and other journals of Elsevier since 2010

Related journal

Local database
Activity: Research › Peer review of manuscripts
A New Active Magnetic Regeneration (AMR) Prototype
Period: 16 Nov 2010
Kurt Engelbrecht (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

European Integrated Center for the Development of New Metallic Alloys and Compounds
15/09/2010 → 18/09/2010
Dresden, Germany
Activity: Talks and presentations › Conference presentations

Oxygen permeation and chemical reactivity of alkaline earth doped cobaltite perovskites for membrane applications: VII Brazilian Electroceramics Symposium
Period: 26 Oct 2010
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
K578
Links:
http://sbpmat.org.br/9encontro/apresentacao/?lang=eng

Related event

IX Brazilian MRS meeting : The Brazilian Materials Research Society
24/10/2010 → 28/10/2010
Minais Gerais, Brazil
Activity: Talks and presentations › Conference presentations

UDTU Education in University Teaching at DTU
Anne Hauch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Participation in module 1-4 (all modules) in UDTU Education in University Teaching at DTU

UDTU - university teachers education

Related event

UDTU Education in University Teaching at DTU
02/08/2010 → 30/06/2011
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

International Symposium on Metal-Hydrogen Systems
Period: 19 Jul 2010 → 23 Jul 2010
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Poster Presentation - Rotational and Translational diffusion in Calcium Borohydride from QENS and DFT

MH2010

Related event

12th International Symposium on Metal-Hydrogen Systems
19/07/2010 → 23/07/2010
Moscow, Russian Federation
Activity: Attending an event › Participating in or organising a conference

Cimtec 2010
Period: 18 Jun 2010
Hanne Lauritzen (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Description
Fabrication and Processing of Polymer and Organic Solar Cells
Documents:
Fabrication and Processing of Polymer and Organic Solar Cells

Related event

Cimtec 2010: 5th Forum on New Materials
13/06/2010 → 18/10/2010
Montecatini Terme, Italy
Activity: Talks and presentations › Conference presentations

EERA Joint Programme on Energy Storage (External organisation)
Period: 1 Jan 2010
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage

Description
European collaboration among universities and research institutiuins

Body type: European
Degree of recognition: International

Related external organisation

EERA Joint Programme on Energy Storage
Activity: Membership › Membership of research networks or expert groups

Udstilling med plastsolceller
Period: 1 Jan 2009
Torben Damgaard Nielsen (Speaker)
Department of Energy Conversion and Storage
Applications, Patents and Innovation
Rise National Laboratory for Sustainable Energy
Solar Energy Programme

Description
Enhedslistens årsmøde

Related external organisation
Enhedslisten
Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Institute of Physics (External organisation)
Period: 2008 → …
Duc-The Ngo (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows
Description
Member
I have been a member of Institute of Physics (IOP, UK) since 2008
Body type: Society
Degree of recognition: International
Related external organisation
Institute of Physics
Beograd
Activity: Membership › Membership of research networks or expert groups

DESIGN OF THE ELECTROCERAMICS FOR SOLID OXIDE FUEL CELL APPLICATIONS: PLAYING WITH CERIA:
Nanotechnology: Controlled Processing of Nanoparticle Structures and Composites
Period: 7 Oct 2008
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
Session: Nanoparticle Sintering II
Related event
Materials Science & Technology Conference and Exhibition: MS&T08
05/10/2008 → 09/10/2008
Pittsburgh, Pennsylvania, United States
Activity: Talks and presentations › Conference presentations

European Fuel Cell Forum (External organisation)
Period: Dec 2007 → Jun 2008
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Scientific Committee
Degree of recognition: International
Related external organisation
European Fuel Cell Forum
Obgardihalde 2, CH-6043, Luzern-Adligenswil, Switzerland
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar
Influence of Sintering on Electrochemical Properties of Nanocrystalline Doped-Ceria: F5 - Nanostructured Metal Oxides: Processing and Applications

Period: 2 Nov 2006
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
Meet. Abstr.-2006-Esposito-1765

Related event
210th ECS meeting, Cancun, Mexico, Oct 29-Nov 3, 2006.
01/01/2006 → ...
Cancun, Mexico
Activity: Talks and presentations › Conference presentations

Prizes:

4th International DHC+ Student Awards - 1st prize
Dominik Franjo Dominkovic (Recipient)
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

Description
The 1st prize award was achieved for a report dubbed "Large scale heat pumps as a link between intermittent electrical energy sources and district heating sector". The evaluation committee awarded three papers. As announced, the prize consists of a research contribution of EUR 1000, presentation of findings at the En+Eff International Trade Fair and Congress for Heating, Cooling and CHP in Frankfurt on 19-20 April 2016 and publishing the article in the International EuroHeat & Power magazine.

Details
Awarded date: Mar 2016
Degree of recognition: International
Granting Organisations: Euroheat & Power international association
Prize: Prizes, scholarships, distinctions

August-Wilhelm Scheer Visiting Professorship@TUM
Tejs Vegge (Recipient)
Department of Energy Conversion and Storage, Atomic scale modelling and materials

Details
Awarded date: 2016
Granting Organisations: Technical University of Munich
Prize: Prizes, scholarships, distinctions

Best Poster Award at the Sustain 2017
Gisele Alves dos Reis Benatto (Recipient), Nicholas Riedel (Recipient), Claire Mantel (Recipient), Sune Thorsteinsson (Recipient), Peter Behrensordofo Poulsen (Recipient), Søren Forchhammer (Recipient), Kenn H. B. Frederiksen (Recipient), Jan Vedde (Recipient), Harsh Parikh (Recipient), Sergiu Sataru (Recipient) & Dezso Sera (Recipient)
Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Coding and Visual Communication, Centre of Excellence for Silicon Photonics for Optical Communications

Description
Outdoor luminescence imaging strategies for drone-based PV array inspection

Details
Awarded date: 6 Dec 2017
Degree of recognition: International
Granting Organisations: Technical University of Denmark
event: Sustain 2017
Prize: Prizes, scholarships, distinctions
Elite-Forsk-rejsestipendium (EliteForsk travel grant)
Dominik Franjo Dominkovic (Recipient)
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

Description
Awarded with the scholarship for the purpose of visiting different research groups. It will be used to finance the guest research stay at Energy Research Institute at Nanyang Technological University in Singapore and for the guest research stay at National Renewable Energy Laboratory (NREL) in Colorado, the USA.

Details
Awarded date: 23 Feb 2017
Degree of recognition: National
Granting Organisations: Ministry of Higher Education and Science
Prize: Prizes, scholarships, distinctions

Ellen and Hans Hermers Award 2015
Tejs Vegge (Recipient)
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials

Description
The Foundation is managed by Rector of the University of Copenhagen, Prof. Ralf Hemmingsen, the Dean of the Faculty of Sciences at University of Copenhagen, Prof. John Renner Hansen, and the President of the Technical University of Denmark, Prof. Anders O. Bjarklev. The foundation awards honorary grants (unsolicited).

Details
Awarded date: 26 Jan 2015
Granting Organisations: Ellen and Hans Hermers Foundation
Prize: Prizes, scholarships, distinctions

Member of the Danish Academy of Technical Sciences (ATV)
Tejs Vegge (Recipient)
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials

Details
Awarded date: May 2014
Granting Organisations: Danish Academy of Technical Sciences (ATV)
Prize: Prizes, scholarships, distinctions

PhD Supervisor the year 2017
Tejs Vegge (Recipient)
Department of Energy Conversion and Storage, Atomic scale modelling and materials

Description
PhD Supervisor of the year at DTU

Details
Awarded date: 27 Oct 2017
Granting Organisations: Technical University of Denmark
Prize: Prizes, scholarships, distinctions

Third Price EFC17 Best Paper Awards
Søren Højgaard Jensen (Recipient), Hendrik Langnickel (Recipient), Nils Hintzen (Recipient), Ming Chen (Recipient), Xiufu Sun (Recipient), Anne Hauch (Recipient), Giacomo Butera (Recipient) & Lasse Rengaard Clausen (Recipient)
Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Department of Mechanical Engineering, Thermal Energy

Description
Third price for the paper: "Reversible Operation using Carbonaceous Gasses of a 30-cell Solid Oxide Cell Stack"

The awards are given to the best papers submitted to the EFC17 conference and that report the most important insights and progress within the broad field of hydrogen and fuel cell technologies. The awards are sponsored by the EFC17
conference. All nominations are judged by an independent Best Paper Selection Committee.

**Details**

Awarded date: 13 Dec 2017  
Degree of recognition: International  
event: 7th EUROPEAN FUEL CELL PIERO LUNGHI CONFERENCE  
Prize: Prizes, scholarships, distinctions

**Press clippings:**

**Nyt batteri kan oplades på ét minut og give 800 km rækkevidde**  
Tejs Vegge  
16/11/2017  
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**The Race to Build Better Batteries**  
Tejs Vegge  
01/11/2017  
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Sådan får du dit batteri til at holde længere**  
Tejs Vegge  
24/10/2017  
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Elektriske fly**  
Tejs Vegge  
16/06/2017  
Atomic scale modelling and materials, Department of Energy Conversion and Storage
Rumforskning: Han skal sikre astronauter en returbillet fra Mars
Christopher R. Graves
17/05/2017

Description
Article in Jyllands Posten about Christopher Graves's involvement in a NASA project that will send a CO2 electrolyzer to Mars on the rover in 2020. Following is the link to the article. A PDF of the full could be uploaded if there was an attachment option.

Applied Electrochemistry, Department of Energy Conversion and Storage

Media coverage (1)

Rumforskning: Han skal sikre astronauter en returbillet fra Mars
17/05/2017
Jyllands Posten (National), Denmark, Print
Lars Dalsgaard
Christopher R. Graves
Press / Media

Batterirevolutionen lader vente på sig
Tejs Vegge
03/05/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Batterirevolutionen lader vente
03/05/2017
Nordea Invest Magasin, Denmark, Web
http://nordeainvestmagasinet.dk/artikler/batterirevolutionen-lader-vente-pa-sig
Tejs Vegge
Press / Media

Mercedes satser stort på produktion af højeffektive batterier
Tejs Vegge
27/04/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Mercedes satser stort på produktion af højeffektive batterier
27/04/2017
DI Energi årsmagasin 2017, Denmark, Web
http://Mercedes satser stort på produktion af højeffektive batterier
Tejs Vegge
Press / Media

Ny kemi i batterier øger muligheden for at lagre grøn energi
Tejs Vegge
20/02/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Ny kemi i batterier øger muligheden for at lagre grøn energi
20/02/2017
Ingeniøren, Denmark, Web
https://ing.dk/artikel/ny-kemi-batterier-oeger-muligheden-at-lagre-groen-energi-193977
Tejs Vegge
**Derfor fryser din mobil sig selv ihjel i kulden**
Tejs Vegge
07/01/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Media contribution (1)**

**Derfor fryser din mobil sig selv ihjel i kulden**
07/01/2017
www.tv2.dk, Denmark, Web
http://livsstil.tv2.dk/forbrug/2017-01-06-derfor-fryser-din-mobil-sig-selv-ihjel-i-kulden
Tejs Vegge
Press / Media

**Ingeniøren - Året Rundt 2016: Lang vej til nye batteriteknologier**
Tejs Vegge
31/12/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Media contribution (1)**

**Ingeniøren - Året Rundt 2016: Lang vej til nye batteriteknologier**
31/12/2016
Ingeniøren, Print
https://ing.dk/artikel/lang-vej-nye-batteriteknologier-190102
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

**DHC+ newsletter: Interview with Dominik Franjo Dominković, winner of the 4th International DHC+ Student Awards**
Dominik Franjo Dominkovic
10/10/2016

**Description**
An interview with the several questions concerning the participation in the DHC+ Student Awards Competition
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

**Media contribution (1)**

**DHC+ newsletter: Interview with Dominik Franjo Dominković, winner of the 4th International DHC+ Student Awards**
10/10/2016
DHC+ Technology Platform, Web
DHC+ Technology Platform
Dominik Franjo Dominkovic
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities
Press / Media

**Eksperter: Samsungs brandfarlige batterier er bekymrende**
Tejs Vegge
11/09/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Media contribution (1)**

**Eksperter: Samsungs brandfarlige batterier er bekymrende**
11/09/2016
www.dr.dk, Web
https://www.dr.dk/nyheder/indland/eksperter-samsungs-brandfarlige-batterier-er-bekymrende
Tejs Vegge
Atomic scale modelling and materials, Department of Energy Conversion and Storage
Press / Media
Bill Gates forgylder tre enegriteknologier
Tejs Vegge
04/12/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Bill Gates med energi nummer 1: Flowbatterier
Tejs Vegge
04/12/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Batterier der virkelig batter
Tejs Vegge
27/10/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)
So ein Ding: Solstrøm og Megabatterier
Tejs Vegge
25/10/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

So ein Ding: Solstrøm og Megabatterier
25/10/2015
DR2, Television
Danmarks Radio
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Efter TESLA: Danske forskere giver deres bud på fremtidens energilagring
Tejs Vegge
18/07/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Efter TESLA: Danske forskere giver deres bud på fremtidens energilagring
18/07/2015
Videnskab.dk, Web
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Fremtidens Energiforsyning
Tejs Vegge
15/06/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Fremtidens Energiforsyning
15/06/2015
NOAHkanalen, Web
https://www.youtube.com/watch?v=tIiNi2v2W63M
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

På falderebet: Siemens ude af el-færgeprojekt
Tejs Vegge
26/05/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

På falderebet: Siemens ude af el-færgeprojekt
26/05/2015
Fyens.dk, Web
Tejs Vegge
Hjemmekraftværk rammer tiden’s and
Tejs Vegge
04/05/2015

Subject
Tesla Powerwall
Department of Physics, Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Hjemmekraftværk rammer tiden’s and
04/05/2015
Berlingske, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics

Nyt batteri kan forsyne dit hus med strøm
Tejs Vegge
01/05/2015
Department of Physics, Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Nyt batteri kan forsyne dit hus med strøm
01/05/2015
TV2 News, Television
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics

Forbedring af batterier er et langt, sejt træk
Tejs Vegge
17/04/2015
Department of Physics, Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Forbedring af batterier er et langt, sejt træk
17/04/2015
 Ingenøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics

Højlunds Helte: Tre DTU’ers løsninger på fremtidens problemer med CO2
Anne Hauch
15/03/2015

Description
Three researchers from DTU Energy participate in the Sunday morning programme ‘Højlund’s Heroes’ on the radio channel Radio24syv. They go live in the radio at 08:25 to approx. 09:00 on Sunday morning, 15 March.

In the programme Højlunds Heroes, PhD student Søren Lyng Ebbehøj, senior researcher Anne Hauch and Professor Jens
Oluf Jensen will talk about the following energy research topic: How do we get fuel in the future?

Højlund’s Heroes is a programme that tells the positive story. The media landscape is fraught with problems, concerns and disasters, but every time there is something to worry about, there are also some ambitious people trying to find the solution. The objective of Højlund’s Heroes is to focus on those people and their work.

Energy is very important in climate perspective and policy perspectives, and many are worried about how we get energy in the future. DTU Energy has been invited to talk about its research in energy technologies, because - as journalist Grethe Højlund says - there’s something inspiring about people moving into the unknown territory to find the solutions of tomorrow.

You can follow our researchers (in Danish) at http://www.radio24syv.dk/programmer/hoejlunds-helte/ this Sunday morning from 08.25 in the morning.

Subject
CO2 capture, electrolysis, fuel cells - Manufacturing Green Fuels from Renewable Energy
Applied Electrochemistry, Department of Energy Conversion and Storage

Media contribution (1)

Højlnuds Helte: Tre DTU'ers løsninger på fremtidens problemer med CO2
15/03/2015
Radio24syv, Radio
Danmarks Radio
25 minutes
The interview of Søren Lyng Ebbehøj, I and Jens Oluf Jensen starts approximately after 24 minutes of the program
Anne Hauch
Department of Energy Conversion and Storage, Applied Electrochemistry
Press / Media

Article in ComputerWorld (DK)
Michael Corazza
02/01/2015
Department of Energy Conversion and Storage, Functional organic materials

Media contribution (1)

Article in ComputerWorld (DK)
02/01/2015
Print
http://www.computerworld.dk/art/232794/risoe-forsker-open-source-er-et-lystvaerk
Michael Corazza
Department of Energy Conversion and Storage, Functional organic materials
Press / Media

Nyt flowbatteri har lovende fremtid
Tejs Vegge
23/06/2014
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Nyt flowbatteri har lovende fremtid
23/06/2014
Ingeniøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Elektrokemi kan ændre vædning mellem metal og keramik: Forskere på DTU Energikonvertering har opdaget, at elektrokemi kan ændre vædningen mellem metal og keramik.
Electrochemistry Unlocks Wettability: Epitaxial Growth of Oxide Nanoparticles on Rough Metallic Surfaces

Anastasia Aleksandrovna Permyakova
01/01/2012

Højeffektive brændselceller
Trine Klemensø
01/01/2010

Description
SOFC project promotion film for The Danish National Advanced Technology Foundation.
Ceramic Engineering & Science, Department of Energy Conversion and Storage

Media contribution (1)
Højeffektive brænselsceller
01/01/2010
Web
Højteknologifonden
10 min
Trine Klemensø
Department of Energy Conversion and Storage, Ceramic Engineering & Science
Press / Media