Complementary analyses of aging in a commercial LiFePO$_4$/graphite 26650 cell

In this work we investigate the electrode degradation mechanisms in a commercial 2.5 Ah LiFePO$_4$/graphite 26650 cylindrical cell. Aged and fresh electrode samples were prepared by cycling two cells respectively five and 22 k times. Subsequently the cells were disassembled in a glovebox and the electrode samples were prepared for electrochemical testing in a 3-electrode setup, and for characterization with XRD, XPS and low-kV FIB/SEM tomography. A 1 μm thick CEI (cathode electrolyte interface) layer was observed at the electrode/electrolyte interface of the aged LiFePO$_4$ electrode. Relative to the fresh LiFePO$_4$ electrode, the aged electrode exhibited a larger series resistance which indicates the observed degradation layer increases the ionic resistance. In addition, micron-sized agglomerates, probably a mixture of carbonaceous material and decomposition products from the electrolyte, were observed at the electrode/electrolyte interface of the aged graphite electrode. These layers may contribute significantly to the loss of lithium inventory (LLI) in the cell, and to the loss of active material (LAM) in the graphite electrode. Low-voltage FIB/SEM tomography was used to detect local charging effects of graphite particles in the carbon electrode, an effect of poor dissipation of the electric charge to the ground after the sample interaction with the electron beam. The charging effects were primarily observed in the aged electrode and most of the locally charged particles were found to be close to the electrode/electrolyte interface, indicating a poorly percolating graphite network near this interface.
Web of Science (2017): Impact factor 5.116
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177
Web of Science (2016): Impact factor 4.798
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.86 SJR 1.321 SNIP 1.324
Web of Science (2015): Impact factor 4.803
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.59 SJR 1.378 SNIP 1.456
Web of Science (2014): Impact factor 4.504
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.44 SJR 1.427 SNIP 1.587
Web of Science (2013): Impact factor 4.086
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.99 SJR 1.644 SNIP 1.574
Web of Science (2012): Impact factor 3.777
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.15 SJR 1.615 SNIP 1.788
Web of Science (2011): Impact factor 3.832
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.685 SNIP 1.715
Web of Science (2010): Impact factor 3.65
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.523 SNIP 1.615
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Scopus rating (2008): SJR 1.524 SNIP 1.458
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.551 SNIP 1.568
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.531 SNIP 1.726
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.484 SNIP 1.516
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.362 SNIP 1.567
Scopus rating (2003): SJR 1.637 SNIP 1.505
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.534 SNIP 1.441
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Scopus rating (2001): SJR 1.312 SNIP 1.376
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.889 SNIP 1.161
Web of Science (2000): Indexed yes
Combined DFT and DEMS investigation of the effect of dopants in secondary zinc-air batteries

Zinc–air batteries offer the potential of low-cost energy storage with high specific energy, but at present secondary Zn–air batteries suffer from poor cyclability. To develop economically viable secondary Zn–air batteries, several properties need to be improved: choking of the cathode, catalyzing the oxygen evolution and reduction reactions, limiting dendrite formation and suppressing the hydrogen evolution reaction (HER). Understanding and alleviating HER at the negative electrode in a secondary Zn–air battery is a substantial challenge, for which it is necessary to combine computational and experimental research. Here, we combine differential electrochemical mass spectrometry (DEMS) and density functional theory (DFT) calculations to investigate the fundamental role and stability when cycling in the presence of selected beneficial additives, that is, In and Bi, and Ag as a potentially unfavorable additive. We show that both In and Bi have the desired property for a secondary battery, that is, upon recharging they will remain on the surface, thereby retaining the beneficial effects on Zn dissolution and suppression of HER. This is confirmed by DEMS, where it is observed that In reduces HER and Bi affects the discharge potential beneficially compared to a battery without additives. Using a simple procedure based on adsorption energies calculated with DFT, it is found that Ag suppresses OH adsorption, but, unlike In and Bi, it does not hinder HER. Finally, it is shown that mixing In and Bi is beneficial compared to the additives by themselves as it improves the electrochemical performance and cyclic stability of the secondary Zn–air battery.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
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Peer-reviewed: Yes

Publication information
Journal: ChemSusChem (Print)
Volume: 11
Issue number: 12
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Impact factor 7.411
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Impact factor 7.226
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 7.33 SJR 2.53 SNIP 1.424
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 7.97 SJR 2.864 SNIP 1.663
Web of Science (2014): Impact factor 7.657
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 6.79 SJR 2.561 SNIP 1.46
Continuous Hydrothermal Flow Synthesis of LaCrO3 in Supercritical Water and Its Application in Dual-Phase Oxygen Transport Membranes

The continuous production of LaCrO3 particles (average edge size 639 nm, cube-shaped) by continuous hydrothermal flow synthesis using supercritical water is reported for the first time. By varying the reaction conditions, it was possible to suggest a reaction mechanism for the formation of this perovskite material. Moreover, dual-phase oxygen transport membranes were manufactured from the as-synthesized LaCrO3 particles and (ZrO2)0.89(Y2O3)0.01(Sc2O3)0.10 (10Sc1YSZ), and oxygen permeation fluxes up to 5 × 10–8 mol cm–2 s–1 were measured on a 1 mm thick membrane.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Pages: 2123-2130
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 57
Issue number: 6
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
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Intercalation of lithium into disordered graphite in a working battery

The structural transformations occurring during the intercalation of lithium into disordered graphite in a working battery were studied in detail by operando X-ray powder diffraction (XRPD). By using a capillary-based micro-battery cell, it was possible to study the stacking disorder in the initial graphite as well as in lithiated graphites. The micro-battery cell was assembled in its charged state with graphite as positive electrode and metallic lithium as counter electrode. The battery was discharged until a stage II compound (LiC12) was formed. The operando XRPD data reveal that the graphitic electrode material retains a disordered nature during the intercalation process. A DIFFaX+ refinement based on the initial operando XRPD pattern shows that the initial graphite generally has an intergrown structure with domains of graphite 2H and graphite 3R. However, the average stacking sequence of the initial graphite also contains a significant concentration of AA-type stacking of the graphene sheets. DIFFaX+ was further used to refine structure models of a stage III type compound and the final stage II compound. The refinement of the stage II compound showed that it is dominated by AαAA-type stacking, but that it also contains a significant concentration of AαABβB-type slabs in the average stacking sequence.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Electrochemical Materials and Interfaces, University of Trento
Contributors: Johnsen, R. E., Norby, P., Leoni, M.
Number of pages: 7
Publication date: 2018
Peer-reviewed: Yes

Publication information

Journal: Journal of Applied Crystallography
Volume: 51
Issue number: 4
ISSN (Print): 0021-8898
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.72 SJR 1.635 SNIP 1.346
Web of Science (2017): Impact factor 3.422
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.221 SNIP 1.211
Web of Science (2016): Impact factor 2.614
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.97 SJR 2.271 SNIP 2.514
Web of Science (2015): Impact factor 2.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.76 SJR 2.564 SNIP 4.297
Web of Science (2014): Impact factor 3.984
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6 SJR 2.934 SNIP 6.334
Correction to Creation of High Mobility Two-Dimensional Electron Gases via Strain Induced Polarization at an Otherwise Nonpolar Complex Oxide Interface

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Center for Electron Nanoscopy, Imaging and Structural Analysis, University of Copenhagen
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 Cu\(_{1+x}\)Mn\(_{2-x}\)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 microstructural 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 CuMn-spinel phase, mixed with a 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
Pages: 730-734
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 5
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Impact factor 2.149
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Impact factor 1.706
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.02 SJR 0.685 SNIP 0.779
Web of Science (2015): Impact factor 1.769
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.05 SJR 0.615 SNIP 0.792
Web of Science (2014): Impact factor 2.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.99 SJR 0.835 SNIP 0.833
Web of Science (2013): Impact factor 1.546
ISI indexed (2013): ISI indexed yes
In this work we characterize all-solid-state lithium-sulfur batteries based on nano-confined LiBH$_4$ in mesoporous silica as solid electrolytes. The nano-confined LiBH$_4$ 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.
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.
Web of Science (2017): Impact factor 2.929
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.82 SJR 1.896 SNIP 1.176
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.59 SJR 1.628 SNIP 1.598
Web of Science (2014): Impact factor 2.436
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Scopus rating (2013): CiteScore 2.66 SJR 1.761 SNIP 1.323
Web of Science (2013): Impact factor 2.745
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.31 SJR 1.866 SNIP 1.562
Web of Science (2012): Impact factor 2.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.35 SJR 1.659 SNIP 1.328
Web of Science (2011): Impact factor 2.471
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.722 SNIP 1.239
Web of Science (2010): Impact factor 2.063
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.755 SNIP 1.544
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.583 SNIP 1.716
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Scopus rating (2006): SJR 1.724 SNIP 1.693
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Scopus rating (2004): SJR 1.482 SNIP 1.69
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Scopus rating (2003): SJR 1.365 SNIP 1.737
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.04 SNIP 1.297
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.52 SNIP 1.195
Scopus rating (2000): SJR 1.351 SNIP 1.058
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.406 SNIP 1.281
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/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
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Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Atomic scale modelling and materials, Northwestern University
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Pages: 259-269
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Power Sources
Volume: 307
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Impact factor 6.945
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
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BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 6.34 SJR 1.9 SNIP 1.667
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 6.3 SJR 1.964 SNIP 2.042
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.63 SJR 1.975 SNIP 2.137
Web of Science (2013): Impact factor 5.211
ISI indexed (2013): ISI indexed yes
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.
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 spectrometric analysis 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
Contributors: Storm, M. M., Christensen, M. K., Younesi, R., Norby, P.
Number of pages: 7
Pages: 21211-21217
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 38
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
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 $H_2O_2$ to $H_2$ 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 $\mu$S/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  
Contributors: Møller-Nilsen, R. E. R., Mølhave, K., Norby, P., Wagner, J. B.  
Number of pages: 112  
Publication date: 2016

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Original language: English  
Electronic versions:  
RolfMollerNilsen_PhD_thesis_1.pdf  
Source: PublicationPreSubmission  
Source-ID: 127629530  

**Magnetic coupling in La(Fe, Mn, Si)$_{13}$H$_y$ within the Bean-Rodbell model**

First order magnetic phase transition materials present a large magnetocaloric effect around the transition temperature, where these materials usually undergo a large volume or structural change. This may lead to some challenges for applications, as the material may break apart during field change, due to high internal stresses. A promising magnetocaloric material is La(Fe, Mn, Si)$_{13}$H$_y$, where the transition temperature can be controlled through the Mn amount. In this work we use XRD measurements to evaluate the temperature dependence of the unit cell volume with a varying Mn amount. The system is modelled using the Bean-Rodbell model, which is based on the assumption that the spin-lattice coupling depends linearly on the unit cell volume. This coupling is defined by the model parameter $\eta$, where for $\eta > 1$ the material undergoes a first order transition and for $\eta \leq 1$ a second order transition. We superimpose a Gaussian 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  
Contributors: Neves Bez, H., Nielsen, K. K., Norby, P., Smith, A., Bahl, C. R. H.  
Number of pages: 7  
Publication date: 2016
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.
Performance and Lifetime Limiting Effects in Li-ion Batteries

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).

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 Li$_2$O$_2$. 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 the thermal 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 Li₂O₂ on the first discharge cycle, the intensity of Li₂O₂ on the second discharge cycle was however diminished. The study furthermore showed how X-rays may affect the Li-O₂ 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 Li₂O₂ which was also 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 coupled 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.

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Contributors: Storm, M. M., Norby, P., Luntz, A. C.
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Rechargeable Lithium-Air Batteries: Investigation of Redox Mediators Using DEMS
The rechargeable aprotic lithium-air battery is a promising technology that offers high theoretical energy density of as much 10 times the capacity of current Li-ion batteries. This type of battery technology differs from conventional batteries because of the gas exchange during discharge/charge cycling. Characterizing the gas content during charge using Differential Electrochemical Mass Spectroscopy (DEMS) allows for in-situ characterization of chemistry in the battery.

Using our DEMS setup we have investigated different cathode materials for lithium-air batteries. A carbon black cathode 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.

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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Contributors: Christensen, M. K., Storm, M. M., Norby, P.
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Publication information
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.
Strain development during the phase transition of La(Fe,Mn,Si)$_{13}$H$_{x}$

We use powder X-ray diffraction to evaluate the temperature dependence of the crystalline properties during the magnetic phase transition of La(Fe,Mn,Si)$_{13}$H$_{x}$ as a function of the Fe/Mn/Si 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.

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Thermo-Chemo-Mechanical Response of Solid Oxide Cells during Reduction and Cooling

General information
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Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Atomic scale modelling and materials, Amminex Emissions Technology A/S
Contributors: Chatzichristodoulou, C., Charlas, B., Kwok, K., Jørgensen, P. S., Norby, P., Hendriksen, P. V., Frandsen, H. L.
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http://ma.ecsdl.org/content/MA2016-01/30/1495.abstract
Source: PublicationPreSubmission
Source-ID: 128053340
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2016

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
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
Contributors: Younesi, R., Christiansen, A. S., Scipioni, R., Ngo, D., Simonsen, S. B., Edström, K., Hjelm, J., Norby, P.
Number of pages: 1
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Peer-reviewed: Yes
Electronic versions:
Analysis_of_the_Interphase.pdf

Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015

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.

Bibliographical note
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Analysis of the Interphase on Carbon Black Formed in High Voltage Batteries

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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Imaging and Structural Analysis, Uppsala University
Contributors: Younesi, R., Christiansen, A. S., Scipioni, R., Ngo, D., Simonsen, S. B., Edström, K., Hjelm, J., Norby, P.
Number of pages: 1
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Electronic versions:
Analysis_of_the_Interphase.pdf

Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015

An Electrochemical Impedance Spectroscopy Investigation of the Overpotentials in Li−O2 Batteries
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Bibliographical note
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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
Contributors: Younesi, R., Christiansen, A. S., Scipioni, R., Ngo, D., Simonsen, S. B., Edström, K., Hjelm, J., Norby, P.
Number of pages: 1
Publication date: 2015
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Electronic versions:
Analysis_of_the_Interphase.pdf

Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015

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.
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.

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Web of Science (2017): Impact factor 9.931
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Web of Science (2016): Impact factor 8.867
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 8.36 SJR 2.62 SNIP 1.643
Web of Science (2015): Impact factor 8.262
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 7.27 SJR 2.331 SNIP 1.514
Web of Science (2014): Impact factor 7.443
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Web of Science (2013): Impact factor
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
Keywords: 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
Charge Localization in the Lithium Iron Phosphate Li$_3$Fe$_2$(PO$_4$)$_3$ at High Voltages in Lithium-Ion Batteries

Possible changes in the oxidation state of the oxygen ion in the lithium iron phosphate Li$_3$Fe$_2$(PO$_4$)$_3$ 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$^{2-}$ 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

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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry
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Pages: 3213-3216
Publication date: 2015
Peer-reviewed: Yes
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.
Original language: English

Keywords: Carboxylate, Chemical solution method, Epitaxial growth, Fluorine-free, Thin films

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10.1109/TASC.2014.2360151
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.

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Scopus rating (2017): CiteScore 13.07
Web of Science (2017): Impact factor 12.08
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Impact factor 12.712
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): Impact factor 13.592
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
Web of Science (2013): Impact factor 12.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 13.78
Web of Science (2012): Impact factor 13.025
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.83
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

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Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.36 SJR 0.211 SNIP 0.244
BFI (2014): BFI-level 1
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Erratum: In Situ Studies of Fe$^{4+}$ Stability in β-Li$_3$Fe$_2$(PO$_4$)$_3$ Cathodes for Li Ion Batteries

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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
Contributors: Christiansen, A. S., Johnsen, R. E., Norby, P., Frandsen, C., Marup, S., Jensen, S. H., Kammer Hansen, K., Holtappels, P.
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Web of Science (2014): Impact factor 3.266
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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.

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Growth of Highly Epitaxial YBa2Cu3O7-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 YBa2Cu3O7-δ (YBCO) films on LaAlO3 (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 conversion 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 Jc 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.

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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.
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...

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In Situ Studies of Fe$^{4+}$ Stability in $\beta$-Li$_3$Fe$_{2}$(PO$_4$)$_3$ Cathodes for Li Ion Batteries
In commercial Fe-based batteries the Fe$^{2+}$/Fe$^{3+}$ oxidation states are used, however by also utilizing the Fe$^{4+}$ oxidation state, intercalation of up to two Li ions per Fe ion could be possible. In this study, we investigate whether Fe$^{4+}$ can be formed and stabilized in $\beta$-Li$_3$Fe$_{2}$(PO$_4$)$_3$. The work includes in situ synchrotron X-ray powder diffraction studies (XRPD) during charging of $\beta$-Li$_3$Fe$_{2}$(PO$_4$)$_3$ 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 Fe$^{4+}$ 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 (O$^-\rightarrow$O$^-$) could possibly explain and charge compensate for the reversible extraction of lithium ions from $\beta$-Li$_3$Fe$_{2}$(PO$_4$)$_3$.

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Erratum in Electrochemical Society. Journal, 2015, 162(6) p. X11: Throughout this paper, the prefix "β-" has been used incorrectly to indicate the rhombohedral phase of Li3Fe2(PO4)3. The material studied in the paper is exclusively the rhombohedral phase and all instances of "β-Li3Fe2(PO4)3" should be replaced with "Li3Fe2(PO4)3."

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 synthesis 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 specie[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. 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]

In Situ X-Ray Diffraction Studies on Structural Changes of a P2 Layered Material during Electrochemical Desodiation/Sodiation
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.

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Web of Science (2013): Indexed yes
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.
Low-voltage FIB/SEM Tomography for 3D Microstructure Evolution of LiFePO$_4$/C Electrode

This work presents an investigation of the degradation mechanisms that occur in LiFePO$_4$/C battery electrodes during charge/discharge cycling. Impedance spectra were measured on a fresh electrode and an electrode aged by cycling. The spectra were modeled with an equivalent circuit which indicates that both the ionic and electronic pathways in the electrode were negatively affected by the cycling. Focused Ion Beam/Scanning Electron Microscopy (FIB/SEM) tomography of both electrodes shows that cycling causes agglomerations of Carbon black (CB). In addition to this, Low-voltage FIB/SEM revealed non-conductive CB in the aged electrode.
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.

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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.49 SJR 2.091 SNIP 1.648
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 stoiciometric 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.

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Structural Investigation of Sodium Layered Oxides Via In Situ Synchrotron X-Ray Diffraction

Sodium layered oxides with mixed transition metals have received significant attention as positive electrode candidates for sodium-ion batteries due to high reversible capacity. Sodium layered oxides would be more promising candidates than lithium-compounds in terms of high stability of MO2 slabs after extraction of Na induced from larger ionic size of Na. In addition, rich crystal chemistry for sodium layered compounds is available since larger Na+ ion is stable in more spacious prismatic site as compared to Li+ ion. In view of this, the phase transformation of layered compounds during electrochemical reaction is generally considered to be a pivotal feature for understanding the relationship between layered structures and electrochemical properties. Here the structure, phase stability, and electrochemical properties of two kinds of layered oxides, P2 and O3, are investigated through in-situ synchrotron XRD experiments. A capillary Na-based cell is designed to minimize interference in other substances such as a separator or external battery parts. This approach could 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.
Thermal decomposition of barium valerate in argon

The thermal decomposition of barium valerate (Ba(C4H9CO2)(2)/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 (Ba(C4H9CO2)(2) decomposes in two main steps, first into BaCO3 with release of C4H9COC4H9 (5-nonanone), whereas final conversion to BaO takes place with release of CO2. 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.
PV-powered lighting systems, light to light systems (L2L), offer outdoor lighting where it is elsewhere cumbersome to enable lighting. Application of these systems at high latitudes, where the difference in day length between summer and winter is large and the solar energy is less requires smart dimming functions for reliable lighting. In this work we have built a laboratory to characterize these systems up to 200 WP from "nose to tail" in great detail to support improvement of the systems and to make accurate field performance predictions.

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A New Look at the Stability of Dimethyl Sulfoxide and Acetonitrile in Li-O2 Batteries

Dimethyl sulfoxide (DMSO) and acetonitrile (MeCN) have recently been highlighted as promising electrolyte solvents for Li-O2 batteries. Possible reactions between these two solvents and Li2O2 are here discussed using X-ray photoelectron spectroscopy to analyze surface of the Li2O2 powder after direct contact with the solvents for different times of exposure. The results indicated that Li2O2 decomposes DMSO solvents, whereas no indication of degradation of MeCN by Li2O2 was observed.

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Scopus rating (2012): SJR 1.068 SNIP 1.006
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Scopus rating (2011): SJR 1.056 SNIP 0.984
Web of Science (2011): Impact factor 1.995
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Communication: The influence of CO₂ poisoning on overvoltages and discharge capacity in non-aqueous Li-Air batteries

The effects of Li₂CO₃ like species originating from reactions between CO₂ and Li₂O₂ at the cathode of non-aqueous Li-air batteries were studied by density functional theory (DFT) and galvanostatic charge-discharge measurements. Adsorption energies of CO₂ at various nucleation sites on a stepped (1 1 0 0) Li₂O₂ surface were determined and even a low concentration of CO₂ effectively blocks the step nucleation site and alters the Li₂O₂ shape due to Li₂CO₃ formation. Nudged elastic band calculations show that once CO₂ is adsorbed on a step valley site, it is effectively unable to diffuse and impacts the Li₂O₂ growth mechanism, capacity, and overvoltages. The charging processes are strongly influenced by CO₂ contamination, and exhibit increased overvoltages and increased capacity, as a result of poisoning of nucleation sites: this effect is predicted from DFT calculations and observed experimentally already at 1% CO₂. Large capacity losses and overvoltages are seen at higher CO₂ concentrations. © 2014 AIP Publishing LLC.

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Web of Science (2014): Impact factor 2.952
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Web of Science (2013): Impact factor 3.122
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.137
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Degradation Studies on LiFePO₄ cathode

Lithium-ion batteries are a promising technology for automotive application, but limited performance and lifetime is still a big issue. The aim of this work is to study and address degradation processes which affect LiFePO₄ (LFP) cathodes - one of the most common cathodes in commercial Li-ion batteries. In order to evaluate how the LFP cathode is affected by C-rate a LFP working electrode, Lithium metal foil counter electrode and Lithium metal reference electrode was tested in a 3-electrode setup with a standard 1M LiPF₆ in 1:1 EC/DMC electrolyte and glass fiber separator. The working electrode/counter electrode was subjected to several charge/discharge cycles between 3.0 V and 4.0 V at different discharge rates. Figure 1 shows the voltage profile of the LFP electrode (solid line) and full battery (dotted line) during charge/discharge process. It is seen that the higher the C-rate, the higher is the polarization furnished by the counter electrode which reduces the capacity. In Figure 2, the discharge capacity [mAh/g] is plotted vs the number of charge/discharge cycles. Series of 10 cycles at a given C-rate was applied to the battery. Each series was followed by a C/10 cycle (green points). A linear fit has been applied to the first series (omitting first two cycles where instability of the system is observed), in order to calculate the degradation rates. High C-rates are seen to affect the discharge capacity, but the capacity is almost completely recovered (green points) and only a limited degradation occurs. Impedance spectroscopy has been also applied to investigate the LFP cathode degradation. Figure 3 shows the imaginary part of the impedance measured at 50% State-of-Charge after each series of cycles. The relative increase in the impedance arc around 1 KHz (assumed to be associated with charge transfer resistance at the LFP particle surfaces) is seen to gradually decrease with increasing number of series. This indicates that more cycles per series is needed to establish a convincing relation between C-rate and degradation. The degradation studies will be coupled with FIB/SEM analysis in order to observe changes in the pore structure or micro cracks that would affect electronic percolation. Figure 4 displays an example of a fresh LFP cathode after FIB cutting. White particles are LFP grains while the black area contains carbon particles and pores, which are difficult to distinguish from each other. Substitution of the epoxy resin with a silicon resin increases the contrast between pores and carbon particles [1] and this will be used in the forthcoming FIB/SEM analysis. References [1] M. Ender et al, Journal of The Electrochemical Society, 159 (7) A972-A980 (2012) [Formula]
and lithium metal for the negative electrode. The electrochemical stability of LiBH$_4$-LiI is found to be limited to 3 V. The all-solid-state cells reach 81% of their theoretical discharge capacity at 60 °C and a discharge rate of 10 μA, but a capacity fade of 1.6% per charge-discharge cycle and a large overvoltage are observed. Impedance spectroscopy results show a strong correlation between changes in the discharge capacity of the cells and changes in the cell resistance over 200 cycles. This may be due to a possible formation of a passivating area in the cell as well as contact issues between the electrode-electrolyte interfaces. The crystal structure and ionic conductivity of the LiBH$_4$-Ca(BH$_4$)$_2$ composite were also studied. No formation of a solid solution is observed and the ionic conductivity is lower than that of pure, ball milled LiBH4. Heat treatment of the samples leads to the formation of a small amount of defect-rich, electronically conducting CaH2 with a cubic crystal structure. Its formation has an effect on the measured conductivity of the samples and increases the risk of an internal short-circuit. This reveals a more general issue that must receive attention in further research on solid electrolytes.

**Impedance perspectives on Li-air battery overpotentials**

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**In Situ Synchrotron XRD on a Capillary Li-O2 Battery Cell**

In situ studies give an opportunity to explore systems with a minimum of external interference. As Li-air batteries hold the promise for a future battery technology the investigation of the discharge and charge components of the cathode and anode is of importance, as these components may hold the key to making a large capacity rechargeable battery[1]. Different design for in situ XRD studies of Li-O2 batteries has been published, based on coin cell like configuration[2] [3] or Swagelok designs [4]. Capillary batteries have been investigated for the Li-ion system since its development[5], but no capillary batteries of Li-air has yet been designed. Some of the advantage of the capillary battery design lies in its ability to separate the cathode and anode and avoid the use of glass fiber or separators, which may enable ex situ analysis of battery components. The battery design consist of a electrolyte filled capillary with anode and cathode in each end suspended on stainless steel wires, the oxygen in-let is placed on the cathode side of the capillary with a flushing system for oxygen in-let. In this study we present a flexible design of a capillary based Li-O2 battery with discharge and charge investigated in dimethoxyethane (DME) with synchrotron XRD. The in situ study in these batteries show clearly how Li2O2 precipitates on the cathode side of the battery during discharge (see Figure), as the Li2O2 reflections at 21.2°, 22.5° and 37.1° grows. The reflection at 27.8, 28.4 and 32.16 is from a stainless steel wire where the cathode is attached. The in situ XRD measurements show how the Li2O2 growth depend on current discharge rate and how the FWHM changes dependent on reflection and charge/discharge. Several cells were tested both ex situ and in situ, and in situ XRD for 1st discharge/charge and 2nd discharge/charge of the battery cell were measured, to give a better understanding of the electrochemistry in the Li-O2 battery. 1. Girishkumar, G., et al.. The Journal of Physical Chemistry Letters, 2010. 1(14): p.
In Situ XRD Investigations on Structural Change of P2-Layered Materials during Electrochemical Sodiation/Desodiation

Sodium layered oxides (NaxMO2) are attractive as positive electrode materials for rechargeable sodium-ion batteries (SIBs) due to high capacity, fast ionic diffusion and simple synthetic process. O3-layered lithium compounds have led successful commercialization of current lithium-ion batteries; as a result, rich experiences for structural studies of O3-layered compounds have been accumulated over the past decades. For sodium layered oxides, however, P2-layered compounds have been reported for better cyclability and structural stability during electrochemical reactions than O3-structure. Therefore, systematic studies on P2-layered materials for SIBs are highly required. In this study, we report the structural and electrochemical property of P2-NaxFeyMnyCo1-2yO2 synthesized by simple solid state reaction. The X-ray diffraction pattern of as-synthesized powder is indexed as a hexagonal lattice (P63/mmc, No.194), which is identical to P2-layered structure. The structural changes in hexagonal P2-layered oxides have been investigated during electrochemical sodiation/desodiation by in-situ synchrotron X-ray diffractions of a capillary based micro battery cell. From the result of in-situ studies, the initial layered structure is maintained from 2.0 to 4.0 V vs. Na+/Na during first desodiation. The phase transformation is observed over the 4.0 V, but the original P2 structure is completely restored at the following sodiation process. The relationship between structural and electrochemical properties of this P2-layered material will be discussed.
Ionic conductivity and the formation of cubic CaH₂ in the LiBH₄–Ca(BH₄)₂ composite

LiBH₄–Ca(BH₄)₂ composites were prepared by ball milling. Their crystal structures and phase composition were investigated using synchrotron X-ray diffraction and Rietveld refinement, and their ionic conductivity was measured using impedance spectroscopy. The materials were found to form a physical mixture. The composites were composed of α-Ca(BH₄)₂, γ-Ca(BH₄)₂ and orthorhombic LiBH₄, and the relative phase quantities of the Ca(BH₄)₂ polymorphs varied significantly with LiBH₄ content. The formation of small amounts of orthorhombic CaH₂ and cubic CaH₂ in a CaF₂-like structure was observed upon heat treatment. Concurrent formation of elemental boron may also occur. The ionic conductivity of the composites was measured using impedance spectroscopy, and was found to be lower than that of ball milled LiBH₄. Electronic band structure calculations indicate that cubic CaH₂ with hydrogen defects is electronically conducting. Its formation along with the possible precipitation of boron therefore has an effect on the measured conductivity of the LiBH₄–Ca(BH₄)₂ composites and may increase the risk of an internal short-circuit in the cells.

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PV led engine characterization lab for standalone light to light systems

PV-powered lighting systems, light-to-light systems (L2L), offer outdoor lighting where it is else where cumbersome to enable lighting. Application of these systems at high latitudes, where the difference in day length between summer and winter is large and the solar energy is low requires smart dimming functions for reliable lighting. In this work we have built a laboratory to characterize these systems up to 200 Wp from “nose to tail” in great details to support improvement of the systems and to make accurate field performance predictions.

General information

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Residual stresses in a co-sintered SOC half-cell during post-sintering cooling

Due to the thermal expansion mismatch between the layers of a Solid Oxide Cell, residual stresses (thermal stresses) develop during the cooling after sintering. Residual stresses can induce cell curvature for asymmetric cells but more importantly they also result in more fragile cells. Depending on the loading conditions, the additional stress needed to break the cells can indeed be smaller due to the initial thermo-mechanical stress state. The residual stresses can for a bilayer cell be approximated by estimating the temperature at which elastic stresses start to build up during the cooling, i.e. the reference temperature (Tref) or the strain difference based on the curvature. This approximation gives good results for bilayers with a defined cooling temperature profile, where the curvature of the bilayer defines a unique balance between the two unknown residual stress states in the two layers. This methodology is however not valid for more layers, as several configurations of residual stresses in the layers can result in the same curvature. Therefore the development of residual stresses of co-sintered multilayer cells during the cooling after sintering is here studied by a finite element model simulation taking into account the elastic response and creep of each layer. The model is validated by measuring the curvature and residual stresses of multi-layer cells.

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Contributors: Charlas, B., Chatzichristodoulou, C., Brodersen, K., Kwok, K., Norby, P., Chen, M., Frandsen, H. L.
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Subsolidus phase relations of the SrO–SbOx–CuO system at 1140K in air

The subsolidus phase relations of the SrO–SbOx–CuO system were investigated in air. The samples were equilibrated at 1140K. Under these conditions, 7 binary oxide phases are stable: Sr2CuO3, SrCuO2, Sr14Cu24O41−δ, CuSb2O6, SrSb2O6, Sr2Sb2O7 and Sr7Sb2O12. The ternary section contains 10 three-phase regions. A new ternary oxide phase with an approximate Sr3Sb2CuO9 composition of was identified. It structure is related to that of Sr8W3CuO18. This phase is not superconducting above 2K. Instead, the magnetic susceptibility indicates onset of weak ferro- or ferrimagnetism at T≈30K.

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Web of Science (2016): Impact factor 3.133
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Scopus rating (2008): SJR 0.888 SNIP 1.21
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.882 SNIP 1.209
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.901 SNIP 1.158
Web of Science (2006): Indexed yes
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Scopus rating (2004): SJR 0.922 SNIP 1.354
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Scopus rating (2002): SJR 0.733 SNIP 1.063
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Scopus rating (2000): SJR 0.707 SNIP 0.938
Temperature- and Pressure-Induced Changes in the Crystal Structure of Sr(NH$_3$)$_{8}$Cl$_2$

ABSTRACT: The structural transformations occurring in the crystal structure of strontium chloride octamine, Sr(NH$_3$)$_8$Cl$_2$, as a function of temperature and pressure of ammonia gas were studied by detailed in situ X-ray powder diffraction (XRPD) and supported by density functional theory (DFT) calculations. Rietveld refinements were used to study the crystal structure of Sr(NH$_3$)$_8$Cl$_2$ in details, and the potential presence of super symmetry is discussed. The Rietveld refinements show that the interatomic distance from the strontium ion to one of the ammonia molecules (Sr–N1) increases from 2.950(7) Å at 275 K to 3.50(6) Å at 322 K at P(NH$_3$) = 2.0 bar. DFT calculations show that only half the energy is required to elongate the Sr–N1 bond from its equilibrium distance compared to the standard Sr–N bonds. The in situ XRPD data show that the a parameter of the unit cell increases relatively more than the b and c parameters during the heating, which is correlated to the crystallographic transformation. The in situ XRPD data show that increasing the heating rate pushes the structural transformation in the crystal structure to higher temperatures by a few kelvin. The in situ XRPD data show that the Sr(NH$_3$)$_8$Cl$_2$ → Sr(NH$_3$)$_2$Cl$_2$ + 6NH$_3$(g) reaction has the lowest transformation temperature for all the studied ammonia pressures. The Sr(NH$_3$)$_8$Cl$_2$ → Sr(NH$_3$)Cl$_2$ + 7NH$_3$(g) reaction also plays a significant role at lower ammonia pressure. For the absorption of ammonia, Sr(NH$_3$)Cl$_2$ + 7NH$_3$(g) → Sr(NH$_3$)$_8$Cl$_2$ was the only observed reaction.
The LiBH₄-LiI Solid Solution as an Electrolyte in an All-Solid-State Battery

The charge and discharge performance of an all-solid-state lithium battery with the LiBH₄-LiI solid solution as an electrolyte is reported. Lithium titanate (Li₄Ti₅O₁₂) was used as the positive electrode and lithium metal as the negative electrode. The performance of the all-solid-state cell is compared with a cell with an identical electrode setup but a liquid electrolyte (1 M LiPF₆ in EC:DMC). All measurements were carried out at a temperature of 60°C. For the all-solid-state cells, 81% of the theoretical discharge capacity is reached for a discharge rate of 10 μA, but a capacity fade of 1.6% per charge-discharge cycle is observed. The electrochemical stability of the LiBH₄-LiI solid solution was investigated using cyclic voltammetry and is found to be limited to 3 V. The impedance of the battery cells was measured using impedance spectroscopy. A strong correlation is found between the change in the discharge capacity of the cells and changes in the cell impedance over 200 charge-discharge cycles. This is expectedly due to the possible formation of passivating areas in the cell and/or loss of contact area between the electrolyte and the electrodes.

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Vacancy ordering and superstructure formation in dry and hydrated strontium tantalate perovskites: A TEM perspective

Crystal structures of Sr4(Sr2Ta2)O11 and Sr4(Sr1.92Ta2.08)O11.12, synthesized by solid state reaction technique in dry and hydrated state have been studied mainly using Transmission Electron Microscopy. Due to the lesser ability of X-rays to probe details in oxygen sublattice, the change in crystal symmetry due to ordering of oxygen vacancies could be detected better using Transmission Electron Microscopy. After detailed analysis through TEM, it was observed that no major change occurs in the cation sublattice. The TEM observations are compared with XRD data and discussed. The crystal symmetries and corresponding unit cells of all the perovskites based on the ordering of oxygen vacancies is deduced. Crystal unit cells based on the observations are proposed with ideal atomic coordinates. Finally an attempt is made to explain the water uptake behaviour of these perovskites based on the proposed crystal structure. © 2014 Elsevier Ltd.

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Scopus rating (2014): CiteScore 2.06 SJR 0.69 SNIP 1.231
Capillary-based micro-battery cell for in situ X-ray powder diffraction studies of working batteries: a study of the initial intercalation and deintercalation of lithium into graphite

A novel capillary-based micro-battery cell for in situ X-ray powder diffraction (XRPD) has been developed and used to study the initial intercalation and deintercalation of lithium into graphite in a working battery. The electrochemical cell works in transmission mode and makes it possible to obtain diffraction from a single electrode at a time, which facilitates detailed structural and microstructural studies of the electrode materials. The micro-battery cell is potentially also applicable for in situ X-ray absorption spectroscopy and smallangle X-ray scattering experiments. The in situ XRPD study of the initial intercalation and deintercalation process revealed marked changes in the diffraction pattern of the graphitic electrode material. After the formation of the solid electrolyte interphase layer, the d spacing of the diffraction peak corresponding to the 002 diffraction peak of graphite 2H changes nearly linearly in two regions with slightly different slopes, while the apparent halfwidth of the diffraction peak displays a few minima and maxima during charging/discharging. DIFFaX+ refinements based on the initial XRPD pattern and the one after the initial discharging–charging cycle show that the structure of the graphite changes from an intergrown structure of graphite 2H and graphite 3R to a nearly ideal graphite 2H structure. DIFFaX+ was also used to refine a model of the stacking disorder in an apparent stage III compound with AaN- and AaAC-type slabs.
Chemical stability of DMSO and ACN solvents in contact with Li$_2$O$_2$

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Combined DFT and Dems Study On the Role of CO2 Poisoning On the Electronic Conduction and Overpotentials in Li-Air Batteries

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Combined XRD and Raman studies of coke types found in SAPO-34 after methanol and propene conversion

We have used a combination of high resolution powder X-ray diffraction (HRPD), Raman spectroscopy, in situ powder diffraction and nitrogen adsorption measurements to study the effect on and nature of coke in the zeotype catalyst SAPO-34 during the methanol to olefin (MTO) and propene oligomerisation (PO) reactions. The coke caused by MTO leads to two distinct sets of HRPD peaks which can be indexed by two SAPO-34 unit cells with different lattice parameters and coke contents. We believe that these unit cells represent different zones of the catalyst filled with different coke types. PO coking does not lead to splitting of the diffraction peaks. Raman spectra show differences between the coke types produced by MTO and PO with the same overall trend of increasingly polyaromatic coke with increasing coke mass. The intensity of the monocyclic and polyaromatic peaks in the MTO Raman spectra correspond to the phase fractions of the two cell types used in the Rietveld refinement, suggesting a link between the two phases and the two coke types. The PO Raman spectra have a stronger polyaromatic band at low coke, suggesting that polyaromatics form faster. In situ powder XRD studies suggest that the C3 feeds do not penetrate the crystallites to the same extent as methanol as the zeolite cages fill with coke. This proposal is supported by nitrogen adsorption measurements.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.6 SJR 1.093 SNIP 1.202
Web of Science (2016): Impact factor 3.615
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.55 SJR 1.184 SNIP 1.168
Web of Science (2015): Impact factor 3.349
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.55 SJR 1.25 SNIP 1.282
Web of Science (2014): Impact factor 3.453
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.39 SJR 1.234 SNIP 1.354
Web of Science (2013): Impact factor 3.209
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.53 SJR 1.496 SNIP 1.57
Web of Science (2012): Impact factor 3.365
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Effect of Heat Treatment on the Lithium Ion Conduction of the LiBH₄–LiI Solid Solution

The LiBH₄–LiI solid solution is a good Li⁺ conductor and a promising crystalline electrolyte for all-solid-state lithium based batteries. The focus of the present work is on the effect of heat treatment on the Li⁺ conduction. Solid solutions with a LiI content of 6.25–50% were synthesized by high-energy ball milling and annealed at 140 °C. Powder X-ray diffraction and scanning electron microscopy were used for characterizing the samples and for comparing their crystallite sizes and the density of defects before and after the annealing. The Li⁺ conductivity was measured using impedance spectroscopy, resulting in conductivities exceeding 0.1 mS/cm at 30 °C and 10 mS/cm at 140 °C. It was found that the formation of defect-rich microstructures during ball milling increased the specific conductivities of these compounds significantly. The phase transition temperatures between the orthorhombic and hexagonal structures of LiBH₄ were measured using differential scanning calorimetry (DSC). The measured transition temperatures range from 100 to −70 °C and show a linear decrease of 70 °C for every 10% of LiI addition up to a LiI content of 25%. The relative stability of the two structures was calculated using density functional theory, and together with the DSC measurements, the calculations were used to evaluate the change in entropic difference between the structures with LiI content.
Electrochemical storage: batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Contributors: Vegge, T., Norby, P.
Pages: 42-46
Publication date: 2013

Host publication information
Title of host publication: DTU International Energy Report 2013: Energy storage options for future sustainable energy systems
Publisher: Technical University of Denmark (DTU)
Editors: Hvidtfeldt Larsen, H., Sønderberg Petersen, L.
ISBN (Print): 978-87-550-3968-1
Electronic versions:
DTU_International_Energy_Report_2013.pdf

ESS Technical Design Report

General information
State: Published
Organisations: Center for Nuclear Technologies, Radioecology and Tracer Studies, Department of Physics, Neutrons and X-rays for Materials Physics, The Hevesy Laboratory, Radiation Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, European Spallation Source ESS AB, University of London, CEA, Helmholtz–Zentrum Berlin für Materialien und Energie, Paul Scherrer Institute, Linköping University, Technical University of Denmark
Number of pages: 690
Publication date: 2013

Publication information
Publisher: European Spallation Source
ISBN (Print): 978-91-980173-2-8
Original language: English
Electronic versions:
TDR_final
Source: PublicationPreSubmission
Source-ID: 110626393
Research output: Research - peer-review › Report – Annual report year: 2013

Frame Stability of Tunnel-Structured Cryptomelane Nanofibers: The Role of Tunnel Cations

The role of tunnel K+ ions on the growth and stability of tunnel-structured cryptomelane-type MnO2 nanofibers (denoted as cryptomelane nanofibers hereafter) has been discussed by means of X-ray diffraction and electron microscopy. Cryptomelane nanofibers with typical diameters of 20–80 nm and lengths of 1–6 μm have been synthesized by means of a simple hydrothermal reaction of KMnO4 and MnSO4 aqueous solutions at 140 °C. The growth of cryptomelane nanofibers under hydrothermal conditions follows a dissolution–recrystallization process and involves a morphological transformation from a layered precursor to the tunnel-structured cryptomelane, in which the K+ ions play important roles in templating and stabilizing the tunneled framework. The presence of tunnel K+ ions also enhances the frame stability of the cryptomelane nanofibers at elevated temperatures. The formation of a layered KxMn2O4 (x ≈ 0.26) with a hexagonal phase structure has been observed at about 900 °C. The transformation from tunneled cryptomelane to layered KxMn2O4 also follows the dissolution–recrystallization growth mechanism, in which the diffusion of K+ ions at high temperatures represents a critical process. The topological correlation between the tunneled and layered MnO2 materials might provide useful information for the synthesis of MnO2 nanomaterials with controlled microstructures for different applications.
In situ powder X-ray diffraction in heterogeneous catalysis

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Contributors: Hansen, J., Norby, P.
Pages: 121-146
Publication date: 2013

Host publication information
Title of host publication: In-situ Characterization of Heterogeneous Catalysts
Publisher: John Wiley & Sons Ltd
Editors: Rodriguez, J. A., Hanson, J. C., Chupas, P. J.
ISBN (Print): 978-1-118-00016-8
URLs:
Research output: Research - peer-review › Book chapter – Annual report year: 2013

In Situ Study of High Voltage Performance of Li$_3$Fe$_2$(PO$_4$)$_3$ Cathodes for Li Ion batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Department of Physics, Experimental Surface and Nanomaterials Physics, Fundamental Electrochemistry
Contributors: Christiansen, A. S., Johnsen, R., Norby, P., Jensen, S. H., Frandsen, C., Mørup, S., Kammer Hansen, K., Holtappels, P.
Pages: 842-842
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2013-02
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
In situ study of high voltage.pdf
Source: dtu
Source-ID: n::oai:DTIC-ART:highwire/390454496::35339
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2013
Reduced Graphene Oxide for Li-Air Batteries: The Effect of Oxidation Time and Reduction Conditions for Graphene Oxide

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Copenhagen
Pages: 472-472
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2013-02
Issue number: 9
ISSN (Print): 2151-2043
Original language: English
Source: dtu
Source-ID: n::oai:DTIC-ART:highwire/390583835::35483
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2013

Simulation Tool for Designing off-Grid PV Applications for the Urban Environments
A barrier for exploiting use of standalone solar lighting for the urban environment seem to be lack of knowledge and lack of available tools for proper dimensioning. In this work, the first part of the development of powerful dimensioning tool is described and initial measurements are presented.

General information
State: Published
Number of pages: 3
Pages: 5CV.7.41
Publication date: 2013

Host publication information
Title of host publication: Proceedings of the 28th EU PVSEC
Electronic versions: 5CV.7.41.pdf
Source: dtu
Source-ID: u::9382
Research output: Research - peer-review › Article in proceedings – Annual report year: 2013

Structure and Magnetic Properties of Cu₃Ni₂SbO₆ and Cu₃Co₂SbO₆ Delafossites with Honeycomb Lattices
The crystal structures of two Delafossites, Cu₃Ni₂SbO₆ and Cu₃Co₂SbO₆, are determined by high-resolution synchrotron powder X-ray diffraction. The Ni and Co are ordered with respect to Sb in the layer of edge sharing octahedra, forming magnetic layers with honeycomb geometry. High-resolution electron microscopy confirms ordering, and selected-area electron diffraction patterns identify examples of the stacking polytypes. Low temperature synthetic treatments result in disordered stacking of the layers, but heating just below their melting points results in nearly fully ordered stacking variants. The major variant in both cases is a monoclinic distortion of a 6-layer Delafosseite polytype, but a significant amount of a 2-layer polytype is also present for the Ni case. The antiferromagnetic ordering with transitions, at 22.3 and 18.5 K for Ni and Co variants, respectively, is investigated by temperature and field dependent magnetization, as well as specific heat. The sharp magnetic transitions support the presence of well developed 2:1 ordering of the Co:Sb or Ni:Sb ions in the honeycomb layers. Neutron diffraction measurements at 4 K are used to determine the magnetic structures. For both the Ni and Co phases, the propagation vector is \( \mathbf{k} = [100] \), and can be described as alternating ferromagnetic chains in the metal-oxide plane giving an overall antiferromagnetic “zigzag” alignment. While orientation of the magnetic moments of the Co is along the b-axis, the Ni moments are in the c-axis plane, approximately parallel to the stacking direction. Bulk magnetization properties are discussed in terms of their magnetic structures.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Princeton University, Max Planck Institute, Oak Ridge National Laboratory, Karlsruhe Institute of Technology, Helmholtz–Zentrum Berlin für Materialien und Energie
The Influence of CO2 Poisoning on Overvoltages and Discharge Capacity in Non-aqueous Li-Air Batteries

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Fundamental Electrochemistry, Applied Electrochemistry
Number of pages: 1
Publication date: 2013
Peer-reviewed: No
Electronic versions:
The_Influence_of_CO2_Poisoning.pdf
Source: dtu
Source-ID: u::9953
Research output: Research › Poster – Annual report year: 2013

Volume of Oxide Vacancies in Fluorite and Perovskite Structured Oxides

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Atomic scale modelling and materials, Mixed Conductors
Contributors: Mogensen, M. B., Norby, P., Chatzichristodoulou, C., Hendriksen, P. V.
Publication date: 2013
Media of output: PowerPoint
Event information
Event: Arthur S. Nowick Memorial Symposium
Location: Kyoto, Japan
Electronic versions:
Volume_of_Oxide_Vacancies.pdf
Research output: Research › Sound/Visual production (digital) – Annual report year: 2013
Plasma properties during RF magnetron sputtering of lithium phosphorous oxynitride thin films

General information
State: Published
Contributors: Stamate, E., Christiansen, A. S., Jensen, S. H., Norby, P., Holtappels, P.
Publication date: 2012

Host publication information
Title of host publication: Proceedings of the Thirteenth International Conference on Plasma Surface Engineering
Research output: Research - peer-review; Article in proceedings – Annual report year: 2012

Resolving the stability and structure of strontium chloride amines from equilibrium pressures, XRD and DFT

Strontium chloride octamine, Sr(NH3)8Cl2, has been shown to be a highly efficient ammonia reservoir for selective catalytic reduction of NOx gases in vehicle exhaust and to hold great potential for indirect hydrogen storage. The possible applications of such metal amines depend explicitly on the conditions for ammonia release and it is thus essential to understand the exact ab- and desorption mechanisms. Here, we apply equilibrium pressure measurements from ammonia desorption, X-ray powder diffraction and density functional theory calculations to identify thermodynamically stable Sr(NH3)Cl2, Sr(NH3)2Cl2 and Sr(NH3)8Cl2 phases. The crystal structures were solved in the space groups Cmcm, Aem2 and Pnma respectively. Controversy regarding the possible existence of a diamine phase is resolved on the basis of a combined structural and thermodynamic analysis of the ammonia release mechanisms, yielding a diamine structure with nearly the same stability as the monoamine. Depending on temperature and pressure, the diamine phase is found to have marginally higher or lower stability than the monoamine phase which explains why the diamine phase is found in some experiments and is not found in others.

General information
State: Published
Pages: 18927-18936
Publication date: 2012
Peer-reviewed: Yes

Publication information
Volume: 37
Issue number: 24
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Impact factor 4.229
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
Web of Science (2016): Impact factor 3.582
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.46 SJR 1.27 SNIP 1.314
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.54 SJR 1.207 SNIP 1.484
Web of Science (2014): Impact factor 3.313
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.38 SJR 1.265 SNIP 1.449
Spin 1/2 Delafossite Honeycomb Compound Cu5SbO6

Cu5SbO6 is found to have a monoclinic, Delafossite-derived structure consisting of alternating layers of O–Cu(I)–O sticks and magnetic layers of Jahn–Teller distorted Cu(II)O6 octahedra in an edge sharing honeycomb arrangement with Sb(V)O6 octahedra. This yields the structural formula Cu(I)3Cu(II)2Sb(V)O6. Variants with ordered and disordered layer stacking are observed, depending on the synthesis conditions. The spin 1/2 Cu2+ ions form dimers in the honeycomb layer. The magnetic susceptibility measured between 5 and 300 K is characteristic of the presence of a singlet–triplet spin gap of 189 K. High resolution synchrotron X-ray diffraction studies indicate that changes in the intra- or interdimer distances between 300 and 20 K, such as might indicate an increase in strength of the Peierls-like distortion through the spin gap temperature, if present, are very small. A comparison to the NaFeO2-type Cu2+ honeycomb compounds Na3Cu2SbO6 and Na2Cu2TeO6 is presented.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Princeton University, SUNY Stony Brook, Delft University of Technology
Subsolidus phase relations of the SrO–WO$_3$–CuO system at 800 °C in air

The subsolidus phase relations of the SrO–WO$_3$–CuO system were investigated in air. The samples were equilibrated at 800 °C. Under these conditions, eight binary oxides are stable. The pseudo-ternary section contains two ternary oxide phases: the previously described Sr$_2$CuWO$_6$ phase as well as a new phase with Sr$_8$CuW$_3$O$_{18}$ stoichiometry. The crystal structure of this new compound was solved and refined in the R-3 space group, unit cell parameters $a = 5.7202$ Å and $c = 28.873$ Å. Sr$_8$CuW$_3$O$_{18}$ has a distorted perovskite type structure, where some of the Sr atoms are positioned at the B sites, and the composition may be given as Sr$_6$(Sr$_2$CuW$_3$)O$_{18}$. There are indications of existence of a superstructure or stacking faults related to Cu/Sr ordering.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy
Contributors: Grivel, J., Norby, P.
Pages: 304-309
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Alloys and Compounds
Volume: 513
ISSN (Print): 0925-8388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.66 SJR 1.02 SNIP 1.403
Web of Science (2017): Impact factor 3.779
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.05 SJR 0.954 SNIP 1.332
Web of Science (2016): Impact factor 3.133
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.03 SJR 0.957 SNIP 1.398
Synthesis, crystal structure and thermal properties of Ca$_6$(C$_{12}$H$_{14}$O$_4$)$_4$(CO$_3$)(OH)$_2$(H$_2$O)$_x$ – a 3D inorganic hybrid material

The inorganic–organic compound Ca$_6$(1,3-adamantanedicarboxylate)$_4$(CO$_3$)(OH)$_2$(H$_2$O)$_x$ with 0 < x < 15.2 was synthesized by hydrothermal methods. The crystal structure was determined on the basis of high resolution synchrotron powder diffraction data and poly-crystal measurements. The crystal structure of Ca$_6$(C$_{12}$H$_{14}$O$_4$)$_4$(CO$_3$)(OH)$_2$(H$_2$O)$_{14}$ is tetragonal, space group I41/amd (141) with a = 29.12 Å, c = 15.85 Å, V = 13 440 Å$^3$ and Z = 8. The compound is classified as a 3D inorganic hybrid material with a 3-dimensional inorganic framework consisting of Ca and O, connected to 1,3-adamantanedicarboxylate anions. The structure shows hydrophilic channels in a diamond-like network. In between the channels there exist hydrophobic pores with surfaces defined by adamantane cages. The shortest distance between hydrogen atoms from different molecules in these pores is 3.6 Å. The largest hydrophilic cavity has a diameter of 10 Å and the pores connecting the channels have a diameter of 5 Å. In the as-synthesised state these channels are filled with water molecules. Reversible dehydration–rehydration occurs. The dehydrated compound easily takes up water from ambient air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Oslo, Norwegian Defence Research Establishment
Contributors: Nielsen, R. B., Norby, P., Kongshaug, K. O., Fjellvåg, H.
Pages: 12082-12089
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Dalton Transactions (Print Edition)
Volume: 41
Issue number: 39
ISSN (Print): 1477-9226
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.93 SJR 1.306 SNIP 0.904
Web of Science (2017): Impact factor 4.099
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.85 SJR 1.229 SNIP 0.918
Web of Science (2016): Impact factor 4.029
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.1 SJR 1.302 SNIP 1.006
Web of Science (2015): Impact factor 4.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064
Web of Science (2014): Impact factor 4.197
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.07 SJR 1.441 SNIP 1.08
Web of Science (2013): Impact factor 4.097
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.79 SJR 1.364 SNIP 0.865
Web of Science (2012): Impact factor 3.806
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.68 SJR 1.163 SNIP 0.751
Web of Science (2011): Impact factor 3.838
The Effect of Microstructure on the Lithium Ion Conduction of the LiBH$_4$-LiI Solid Solution

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry
Contributors: Sveinbjörnsson, D. P., Blanchard, D., Mogensen, M. B., Norby, P., Vegge, T.
Number of pages: 1
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from Pacific Rim Meeting on Electrochemical and Solid-State Science, Honolulu, United States.
Source: PublicationPreSubmission
Source-ID: 117919791
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Exfoliation and thermal transformations of Nb-substituted layered titanates

Single-layer Nb-substituted titanate nanosheets of ca. 1 nm thickness were obtained by exfoliating tetrabutylammonium (TBA)-intercalated Nb-substituted titanates in water. AFM images and turbidity measurements reveal that the exfoliated nanosheets crack and corrugate when sonicated. Upon heating, the thermal transformation into anatase and further to rutile is retarded. This suppression of the phase transition upon higher valent substitution may promote technological applications of anatase thin films, hereunder development of films with TCO properties. Depending on the oxygen partial pressure during the transformation, the Nb-substitution into TiO$_2$ provokes different defect situations and also electronic properties. At reducing conditions, Nb is incorporated as NbV and an equivalent amount of TiIV is transformed to TiIII as evidenced by XPS. Magnetic susceptibility data show accordingly paramagnetic behavior. For samples heated in air TiIV and NbV cations prevail, the latter is compensated by cation vacancies. 93Nb MAS NMR data prove that Nb is finely dispersed into the transformed (Ti,Nb)O$_2$ oxide matrices without sign of Nb$_2$O$_5$ (nano)precipitates. The Nb–O–Ti bonds
and defects at cation sites are considered key factors for increasing the transformation temperatures for conversion of the nanosheets to anatase and finally into rutile. It is further tempting to link the delay in crystallization to morphology limitations originating from the nanosheets. The present work shows that layered Nb-titanates are appropriate precursors for formation of highly oriented Nb-substituted anatase thin films via delamination, reconstruction and subsequent heat treatment.

**General information**

State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, University of Oslo, SINTEF
Pages: 3135-3143
Publication date: 2011
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Solid State Chemistry
Volume: 184
Issue number: 12
ISSN (Print): 0022-4596
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 2.2 SJR 0.632 SNIP 0.805
- Web of Science (2017): Impact factor 2.179
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.09 SJR 0.618 SNIP 0.871
- Web of Science (2016): Impact factor 2.299
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 2.18 SJR 0.679 SNIP 0.956
- Web of Science (2015): Impact factor 2.265
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): CiteScore 2.35 SJR 0.799 SNIP 1.058
- Web of Science (2014): Impact factor 2.133
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): CiteScore 2.22 SJR 0.769 SNIP 1.036
- Web of Science (2013): Impact factor 2.2
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): CiteScore 2.27 SJR 0.931 SNIP 1.184
- Web of Science (2012): Impact factor 2.04
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): CiteScore 2.5 SJR 1.004 SNIP 1.299
- Web of Science (2011): Impact factor 2.159
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.068 SNIP 1.202
- Web of Science (2010): Impact factor 2.261
Combined XRD and XANES studies of a Re-promoted Co/γ-Al2O3 catalyst at Fischer–Tropsch synthesis conditions

A cobalt based Fischer–Tropsch catalyst was studied during the initial stages of the reaction at industrially relevant conditions. The catalyst consists of 20wt% cobalt supported on γ-Al2O3 and promoted by 1wt% of rhenium. X-ray diffraction (XRD) in combination with X-ray absorption near edge structure (XANES) were used to reveal information on the particle and crystallite size and the oxidation states of the active component. Conditions giving high selectivity towards light hydrocarbons (methanation, 673K, 10bar and high GHSV) were compared to conditions were higher hydrocarbons are the main products (FT synthesis at 483K, 18bar and low GHSV). The data analysis shows no significant changes in the cobalt crystallites during the first hours of Fischer–Tropsch synthesis. Running the reaction at higher temperatures and predominantly methanation conditions led to significant sintering of the cobalt particles and a further reduction of a partially reduced catalyst could be observed.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Norwegian University of Science and Technology, Statoil ASA
Contributors: Rønning, M., Tsakoumis, N. E., Voronov, A., Johnsen, R., Norby, P., van Beek, W., Borg, Ø., Rytter, E., Holmen, A.
Pages: 289-295
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Catalysis Today
Volume: 155
Issue number: 3-4
ISSN (Print): 0920-5861
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.55 SJR 1.347 SNIP 1.329
Web of Science (2017): Impact factor 4.667
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
Web of Science (2016): Impact factor 4.636
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4 SJR 1.335 SNIP 1.403
Web of Science (2015): Impact factor 4.312
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.72 SJR 1.315 SNIP 1.453
Web of Science (2014): Impact factor 3.893
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.39 SJR 1.299 SNIP 1.415
Web of Science (2013): Impact factor 3.309
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.38 SJR 1.469 SNIP 1.422
Web of Science (2012): Impact factor 2.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.34 SJR 1.472 SNIP 1.562
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.761 SNIP 1.449
Web of Science (2010): Impact factor 2.993
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.718 SNIP 1.631
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.692 SNIP 1.533
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.595 SNIP 1.594
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.512 SNIP 1.346
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.632 SNIP 1.739
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.686 SNIP 1.831
Scopus rating (2003): SJR 1.868 SNIP 1.781
Scopus rating (2002): SJR 1.646 SNIP 1.531
Scopus rating (2001): SJR 1.859 SNIP 1.683
Scopus rating (2000): SJR 1.215 SNIP 1.545
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.373 SNIP 1.437
DIFFaX+ study of stacking disorder in a mixed oxide

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy
Contributors: Johnsen, R., Norby, P.
Publication date: 2010
Peer-reviewed: No
Keywords: Batteries and carbon-free energy storage, Materials and energy storage
Source: orbit
Source-ID: 268620
Research output: Research › Poster – Annual report year: 2010

High energy synchrotron X-ray diffraction studies of lithium batteries

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy
Contributors: Norby, P., Vegge, T., Abrahamsen, A. B., Pedersen, A. S., Zimmermann, M. V.
Publication date: 2010
Peer-reviewed: No
Keywords: Batteries and carbon-free energy storage, Materials and energy storage
Source: orbit
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High performance lithium batteries for transportation: In situ synchrotron X-ray diffraction studies

General information
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Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy
Contributors: Norby, P.
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Research output: Research › Conference abstract for conference – Annual report year: 2010

Structural and microstructural changes during anion exchange of CoAl layered double hydroxides: an in situ X-ray powder diffraction study

Anion-exchange processes in cobalt-aluminium layered double hydroxides (LDHs) were studied by in situ synchrotron X-ray powder diffraction (XRPD). The processes investigated were CoAl-CO3 CoAl-Cl, CoAl-CO3 CoAl-NO3, and CoAl-CO3 CoAl-SO4. The XRPD data show that the CoAl-CO3 phase decreases exponentially while that of the CoAl-Cl phase increases exponentially. Energy-dispersive X-ray spectroscopy (EDXS) studies of a partially chloride-exchanged CoAl-CO3 LDH sample along with in situ XRPD data suggested that the individual particles in the CoAl-CO3 sample are generally anion-exchanged with chloride one at a time. In contrast with the CoAl-CO3 CoAl-Cl transformation, the XRPD data show that the reverse CoAl-Cl CoAl-CO3 process is a one-phase transformation. Rietveld refinements indicate that the occupancy factors of the carbon and oxygen sites of the carbonate group increase, while that of the chloride site decreases. In the CoAl-Cl CoAl-NO3 anion-
exchange reaction, the XRPD patterns reveal the existence of two intermediate phases in addition to the initial CoAl-Cl and final CoAl-NO3 phases. The in situ data indicate that one of these intermediates is a mixed nitrate- and chloride-based LDH phase, where the disorder decreases as the nitrate content increases. The XRPD data of the partial CoAl-CO3 CoAl-SO4 anion-exchange reaction show that the process is a two-phase transformation involving a sulfate-containing LDH with a 1H polytype structure.

**General information**
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Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Swiss Federal Institute of Technology
Contributors: Johnsen, R., Krumeich, F., Norby, P.
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Volume: 43
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.72 SJR 1.635 SNIP 1.346
Web of Science (2017): Impact factor 3.422
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.221 SNIP 1.211
Web of Science (2016): Impact factor 2.614
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.97 SJR 2.271 SNIP 2.514
Web of Science (2015): Impact factor 2.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.76 SJR 2.564 SNIP 4.297
Web of Science (2014): Impact factor 3.984
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6 SJR 2.934 SNIP 6.334
Web of Science (2013): Impact factor 3.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.67 SJR 2.58 SNIP 4.659
Web of Science (2012): Impact factor 3.343
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.32 SJR 3.818 SNIP 3.874
Web of Science (2011): Impact factor 5.152
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.626 SNIP 2.056
Web of Science (2010): Impact factor 3.794
Syntheses, Crystal Structures, and Thermal Stabilities of Polymorphs of Cr(thd)3

The syntheses, crystal structures, and thermal stabilities of six polymorphs of Cr(thd)3 [\(\text{thd}^-\) = anion of H(thd) = C11H20O2 = 2,2,6,6-tetramethylheptane-3,5-dione] were studied using X-ray diffraction and differential scanning calorimetry. Compound 1 is thermodynamically stable below ca. 110 °C and forms plate-shaped crystals \([a = 9.927(5), b = 18.010(5), c = 21.427(5) \text{ Å}, \text{and } \beta = 95.461(5)^\circ \text{ at } 295 \text{ K}; \text{space group } C2/c]\). Its crystal structure is isotypic with Mn(thd)3.

Polymorph 4 is metastable to 1, and the only way to prepare 4 appears to be by precipitation from solution. Crystals of 4 are needle shaped \([a = 28.54(3), b = 19.14(2), c = 21.92(2) \text{ Å}, \text{and } \beta = 97.31(2)^\circ \text{ at } 295 \text{ K}; \text{space group } C2/c]\) and this structure is isotypic with monoclinic Co(thd)3. Modifications 2, 2*, and 5 also appear as needle-shaped crystals \([\text{orthorhombic: } a = 18.97(7), b = 18.69(7), \text{ and } c = 10.62(5) \text{ Å for 2 and tetragonal: } a = b = 18.93(5) \text{ and } c = 10.57(4) \text{ Å for 5, both at } 110 \text{ K}]\). Crystals of 2 and 5 have limited lifetime, which depends on storage conditions and exposure to X-rays. The conversion sequence is: 5 \(\rightarrow\) 2 \(\rightarrow\) 1, where the first step takes 3 to 4 h and the second some 20 h. Attempts to establish detailed accounts of the orthorhombic Co(thd)3-type structure of 2 and 2* by SXD were unsuccessful due to disorder. The structural distinction between 2 and 2* appears to be associated with rotational disorder among the Cr(thd)3 molecules. 2* and 3 are high-temperature modifications with stability range ca. 155–200 and ca. 200–235 °C, respectively [Cr(thd)3 melts at ca. 235 °C]. Quenched 2* can be retained as metastable at room temp. for some weeks, whereas 3 is not quenchable. High-temperature PXD data show that 3 is cubic \([a = 13.357(4) \text{ Å at } 225 \text{ °C}; \text{with strong rotational disorder of the molecules}]\). There are only minor variations in bond lengths and angles between 1 and 4 or from 100 to 295 K, and disorder is limited.
Issue number: 13-14
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.18 SJR 0.411 SNIP 0.461
Web of Science (2017): Impact factor 1.179
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.09 SJR 0.409 SNIP 0.429
Web of Science (2016): Impact factor 1.144
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.22 SJR 0.454 SNIP 0.537
Web of Science (2015): Impact factor 1.261
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.06 SJR 0.409 SNIP 0.552
Web of Science (2014): Impact factor 1.16
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.18 SJR 0.416 SNIP 0.547
Web of Science (2013): Impact factor 1.251
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.15 SJR 0.484 SNIP 0.562
Web of Science (2012): Impact factor 1.163
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.22 SJR 0.481 SNIP 0.554
Web of Science (2011): Impact factor 1.249
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.51 SNIP 0.556
Web of Science (2010): Impact factor 1.247
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.446 SNIP 0.608
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.576 SNIP 0.835
Scopus rating (2007): SJR 0.651 SNIP 0.829
Scopus rating (2006): SJR 0.665 SNIP 0.786
Scopus rating (2005): SJR 0.567 SNIP 0.741
Scopus rating (2004): SJR 0.493 SNIP 0.67
Scopus rating (2003): SJR 0.524 SNIP 0.737
Scopus rating (2002): SJR 0.7 SNIP 0.866
Scopus rating (2001): SJR 0.709 SNIP 0.847
Scopus rating (2000): SJR 0.691 SNIP 0.904
Scopus rating (1999): SJR 0.72 SNIP 0.969
Original language: English
DOIs:
10.1002/zaac.201000160
Source: orbit
Source-ID: 276936
Research output: Research - peer-review › Journal article – Annual report year: 2010
Synthesis and Properties of Layered-Structured Mn5O8 Nanorods

Mn5O8 nanorods were prepared by a topotactic conversion of γ-MnOOH nanorod precursors in nitrogen at 400 °C. The as-prepared Mn5O8 nanorods crystallized in a monoclinic structure (space group C2/m) with unit cell dimensions $a = 10.3784(2)$ Å, $b = 5.7337(7)$ Å, $c = 4.8668(6)$ Å, and $\beta = 109.491(6)^\circ$, having a compositional formula Mn22+Mn34+O8. The structure allowed 18 Raman-active modes (10 Ag + 8 Bg); 10 of these contributions were observed at 262, 300, 391, 429, 475, 533, 576, 615, 647, and 789 cm$^{-1}$. An intensive Ag mode at 647 cm$^{-1}$ was identified, representing a clear signature for probing the Mn5O8 materials via Raman scattering. X-ray photoelectron spectroscopy studies revealed the distinctive spectral features of the Mn5O8 due to the coexistence of divalent and tetravalent Mn ions. Magnetic measurements confirmed further that Mn5O8 was a mixed valence oxide with an antiferromagnetic transition at about 133 K. The decreased Nel temperature of the Mn5O8 nanorods suggested the possible presence of the finite size effect, which accounted also for the red-shift of the corresponding Raman bands in comparison with those of the bulk counterparts.
The adsorption of methanol and water on SAPO-34: in situ and ex situ X-ray diffraction studies

The adsorption of methanol on SAPO-34 has been studied using a combination of in situ synchrotron powder X-ray diffraction to follow the process and ex situ high resolution powder diffraction to determine the structure. The unit cell volume of SAPO-34 is found to expand by 0.5% during methanol adsorption displaying greater flexibility than silicalite under similar conditions. When water is adsorbed onto the framework it contracts, while the non-polar polymethylbenzene intermediates in the methanol to olefin process cause a significant expansion. We therefore suggest that the expansion (water < methanol < polymethylbenzenes) is linked to the strength of interaction with the framework and size of the adsorbent. The position of the methanol molecule has been determined from high resolution powder diffraction data. The oxygen to framework contacts are slightly longer than reported elsewhere for adsorbed water molecules on the same framework, supporting the observation from the in situ data that water is more strongly bound than methanol. The results are consistent with previous results from thermodynamic and tapered element oscillating microbalance measurements.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, University of Oslo
Contributors: Wragg, D. S., Johnsen, R., Norby, P., Fjellwåg, H.
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Publication information
Journal: Microporous and Mesoporous Materials
Volume: 134
Issue number: 1-3
ISSN (Print): 1387-1811
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
A comparison study on Raman scattering properties of alpha- and beta-MnO2

In this comment to a recent paper [Anal. Chim. Acta 585 (2007) 241–245], we report a comparison study on Mn oxide-related compounds with different crystallographic forms, which distinguish between β-MnO2 and α-MnO2 type materials via Raman scattering (RS) spectroscopy. The tetragonal rutile-type β-MnO2 is characterized by a RS band at 667 cm⁻¹ of symmetry A1g, whereas the α-MnO2 type materials feature two main RS contributions at about 574 and 634 cm⁻¹, belonging to Ag spectroscopic species of a tetragonal hollandite-type framework. These data represent a clear signature for identifying β-MnO2 and α-MnO2 type materials via RS spectroscopy.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, University of Oslo
Contributors: Gao, T., Fjellvåg, H., Norby, P.
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Publication date: 2009
Peer-reviewed: Yes

Publication Information
Journal: Analytica Chimica Acta
Volume: 648
Issue number: 2
ISSN (Print): 0003-2670
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.06
Web of Science (2017): Impact factor 1.363
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.01
Web of Science (2016): Impact factor 1.74
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.94
Web of Science (2015): Impact factor 1.682
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.64
Web of Science (2014): Impact factor 2.003
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.74
Web of Science (2013): Impact factor 1.547
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.55
Web of Science (2012): Impact factor 1.747
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.62
Web of Science (2011): Impact factor 1.65
A Structural Study of Stacking Disorder in the Decomposition Oxide of MgAl Layered Double Hydroxide: A DIFFaX plus Analysis

The structure of the decomposition oxide of a nitrate-based magnesium-aluminum layered double hydroxide (LDH) was studied in detail by means of the DIFFaX+ refinement program. The DIFFaX+ refinement was based on in situ X-ray powder diffraction pattern (XRPD) collected at 890 degrees C and showed that the decomposition oxide is a disorder phase, where periclase-type layers and spinel-OT-type layers with different cation concentration and distribution are stacked along the direction corresponding to the cube diagonal of the ideal cubic periclase and/or spinel structure. The spinel-OT-type layers in the periclase-like decomposition phase are assumed to contain significant amounts of tetrahedrally coordinated aluminum atoms. Furthermore, the DIFFaX+ refinement of the decomposition oxide indicated that the octahedra and tetrahedra of the spinel-OT-type layer and the octahedra of some of the periclase-type layer are distorted due to deviation in the cubic-close packing of the oxygen atoms in the decomposition oxide. Our detailed structural investigation described the disorder present in the periclase-like decomposition oxide and revealed the origin of an additional major diffraction peak in the powder diffraction pattern which has up to now remained unexplained.
Conductivity and water uptake of Sr₄(Sr₂Nb₂)O₁₁·nH₂O and Sr₄(Sr₂Ta₂)O₁₁·nH₂O

The hydrated oxygen deficient complex perovskite-related materials Sr₄(Sr₂Nb₂)O₁₁·nH₂O and Sr₄(Sr₂Ta₂)O₁₁·nH₂O were studied at high water vapour pressures over a large temperature range by electrical conductivity measurements, thermogravimetry (TG), and X-ray powder diffraction (XRPD). In humid
atmospheres both materials are known to exhibit protonic conductivity below dehydration temperatures, with peak-shaped maxima at about 500 degrees C. In this work we show that the peaks expand to plateaus of high conductivity from 500 to 700 degrees C at a water vapour pressure of 1 atm. However, in situ synchrotron XRPD of Sr-4(Sr2Nb2)O-11 center dot nH(2)O as a function of temperature shows that these observations are in fact coincident with melting and dehydration of a secondary phase Sr(OH)(2). The stability of Sr-4(Sr2Nb2)O-11 center dot nH(2)O and Sr-4(Sr2Ta2)O-11 center dot nH(2)O in humid atmospheres is thus insufficient, causing decomposition into perovskites with lower Sr content and SrO/Sr(OH)(2) secondary phases. This, in turn, rationalizes the observation of peaks and plateaus in the conductivity of these materials. (C) 2009 Elsevier B.V. All rights reserved.
Crystal Structures of Titanate Nanotubes: A Raman Scattering Study

Crystal structures of titanate nanotubes prepared from a NaOH treatment of TiO2 with subsequent acid washing were discussed from a viewpoint of vibrational spectroscopy. The correlation between the vibrational feature and the polymerization nature of the TiO6 octahedron was established by analyzing Raman scattering data of crystalline TiO2 (anatase and rutile) and layered protonic titanates. Then, the polymerization nature of TiO6 octahedra in the titanate nanotubes was identified by comparing their Raman scattering spectra with those of the crystalline TiO2 and layered protonic titanates. It demonstrated that the titanate nanotubes consist of two-dimensional TiO6 octahedral host layers with a lepidocrocite (gamma-FeOOH)-type layered structure. This conclusion was confirmed further by considering the Raman scattering properties of a restacked titanate prepared by assembling TiO6 octahedral layers derived from the original scroll-like titanate nanotubes. Our findings offered a convenient approach to validate the crystal structures of the products from an alkaline treatment of TiO2 under different experimental conditions.

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Organisations: University of Oslo
Contributors: Gao, T., Fjellvåg, H., Norby, P.
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Peer-reviewed: Yes

Publication information
Journal: Inorganic Chemistry
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ISSN (Print): 0020-1669
Ratings:
BFI (2018): BFI-level 2
Defect Chemistry of a Zinc-Doped Lepidocrocite Titanate CsxTi2−x/2Znx/2O4 (x = 0.7) and its Protonic Form

A zinc-doped layered titanate CsxTi2−x/2Znx/2O4 (x = 0.7) with lepidocrocite (γ-FeOOH)-type layered structure was prepared via solid-state calcination. A complete extraction of both lattice Zn atoms and interlayer Cs ions was observed upon acid exchange, producing a protonic form H2xTi2−x/2x/2O4·H2O that inherited the original lepidocrocite-type layered structure. This new phase was distinguished from its isomorphous related compounds in terms of high proton content, high charge density, and high defect content as a consequence of extractable Zn atoms located in the host framework. The protonic titanate H2xTi2−x/2x/2O4·H2O readily underwent delamination to produce its molecular single sheets Ti1−δδO24δ− (δ = 0.175) with distinctive two-dimensional morphology and small thickness (1 nm), suggesting promising applications in the assembly of functional nanostructures.

General information
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Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, University of Oslo
Contributors: Gao, T., Fjellvåg, H., Norby, P.
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Peer-reviewed: Yes

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Journal: Chemistry of Materials
Volume: 21
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 9.74 SJR 4.675 SNIP 1.896
Web of Science (2017): Impact factor 9.89
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.89 SJR 4.136 SNIP 1.883
Web of Science (2016): Impact factor 9.466
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 9.38 SJR 3.958 SNIP 2.061
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.89 SJR 3.595 SNIP 2.222
Web of Science (2014): Impact factor 8.354
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 8.94 SJR 3.666 SNIP 2.267
Efficient Complete Oxidation of Acetaldehyde into CO2 Over Au/TiO2 Core-Shell Nano Catalyst Under UV and Visible Light Irradiation

Photocatalytic degradation of acetaldehyde and its photocatalytic mechanisms over Au/TiO2 core-shell nano catalyst were, for the first time, investigated under UV and visible light irradiation. The results indicate that Au/TiO2 core-shell catalyst shows higher activity for the oxidation of acetaldehyde into CO2 under both UV and visible light irradiation comparing with P-25 and metal-deposited TiO2 photocatalysts. When Au/TiO2 core-shell catalyst is excited by UV light, the Au-core acts as the sink to restore the separated electrons, thus to improve the photoinduced charge separation; while under visible light irradiation, the mechanism can be understood as the coordinate effect of the plasmon resonance of Au-core particles and the formation of an impurity energy level induced by TiO2-xFx.
In situ studies of structural stability and proton conductivity of titanate nanotubes
Titanate nanotubes were prepared by hydrothermal treatment of anatase TiO2 with concentrated NaOH solution. In situ synchrotron X-ray diffraction studies revealed that the nanotubes are thermally unstable at temperatures above 360 degrees C and can transform directly to anatase via a dehydration and recrystallization process. This indicated that the titanate nanotubes possess an orthorhombic lepidocrocite (gamma-FeOOH)-type layered structure. An aggregate of the as-prepared nanotubes showed an electric conductivity of about 1 x 10(-6) S cm(-1) at 50 degrees C in humid atmospheres. The conductivity depended on humidity of the atmosphere and decreased with increasing temperatures, suggesting that the proton conduction in the titanate nanotubes might correlate with the interlayer H3O+ ions.

General information
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Contributors: Gao, T., Fjeld, H., Fjellvåg, H., Norby, T., Norby, P.
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Peer-reviewed: Yes

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Journal: Energy & Environmental Science
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 30.87 SJR 14.59 SNIP 4.819
Web of Science (2017): Impact factor 30.067
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
Web of Science (2016): Impact factor 29.518
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): CiteScore 19.28 SJR 7.769 SNIP 4.001
Web of Science (2014): Impact factor 20.523
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 14.81 SJR 6.019 SNIP 2.996
Web of Science (2013): Impact factor 15.49
Microstructures, Surface Properties and Topotactic Transitions of gamma-MnOOH Nanorods

Single crystalline monoclinic Manganite (gamma-MnOOH) nanorods have interesting surface properties and thermal behaviors that are distinctive from those of the bulk counterparts.

General information
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Organisations: Swiss Federal Institute of Technology Zurich, University of Oslo
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.7 SJR 1.892 SNIP 1.123
Web of Science (2017): Impact factor 4.7
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.804 SNIP 1.199
Web of Science (2016): Impact factor 4.857
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.7 SJR 1.782 SNIP 1.229
Web of Science (2015): Impact factor 4.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.69 SJR 1.867 SNIP 1.306
Preparation of Nb-Substituted Titanates by a Novel Sol-Gel Assisted Solid State Reaction

Single-phase layered Nb-substituted titanates, Na2Ti3-xNbxO7 (x = 0-0.06) and Cs0.7Ti1.8-xNbxO4 (x = 0-0.03), were for the first time synthesized by a novel sol-gel assisted solid state reaction (SASSR) route. Conventional solid state reactions as well as sol-gel synthesis did not succeed in producing phase pure Nb-substituted titanates. In the SASSR
synthesis route we combine the advantages of traditional sol-gel technique (i.e., homogeneous products formed at low temperatures) and solid state reaction (i.e., formation of stable, crystalline phases) for preparing single-phase niobium-substituted layered titanates. The obtained products were characterized by X-ray powder diffraction, scanning electron microscopy, inductively coupled plasma-atomic emission spectrometry, Raman spectroscopy, and thermogravimetric analysis. Results indicate that the Ti(IV) in the host layer of the samples could be partially replaced by Nb(V) without structural deterioration. After proton-exchange, more water molecules were intercalated into the interlayer of H0.7Ti1.8-xNbxO4 center dot nH(2)O with increasing niobium content, whereas the interlayer distance of H2Ti3-xNbxO7 (x = 0-0.06) was unchanged.

General information
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.7 SJR 1.892 SNIP 1.123
Web of Science (2017): Impact factor 4.7
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.804 SNIP 1.199
Web of Science (2016): Impact factor 4.857
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.7 SJR 1.782 SNIP 1.229
Web of Science (2015): Impact factor 4.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.69 SJR 1.867 SNIP 1.306
Web of Science (2014): Impact factor 4.762
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.9 SJR 1.821 SNIP 1.368
Web of Science (2013): Impact factor 4.794
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.72 SJR 2.094 SNIP 1.341
Web of Science (2012): Impact factor 4.593
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.64 SJR 1.921 SNIP 1.313
Web of Science (2011): Impact factor 4.601
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.006 SNIP 1.309
Protonic titanate derived from CsxTi2-x/2Mgx/2O4 (x=0.7) with lepidocrocite-type layered structure

A layered titanate CsxTi2-x/2Mgx/2O4 (x = 0.7) with lepidocrocite (gamma-FeOOH)-type layered structure was prepared via solid-state reaction. Extraction of both Mg2+ ions in the host layers and interlayer Cs+ ions was achieved during an acid-exchange process, producing a new protonic titanate HxTi2-x/2O4-x/2 \cdot H2O. This phase was distinguished from isomorphous related compounds in terms of removable lattice Mg and O atoms. The protonic titanate HxTi2-x/2O4-x/2 center dot H2O showed excellent exfoliation/delamination reactivity upon intercalating organic amine ions as well as the ability to produce single two-dimensional titanate nanosheets with small thickness of about 1 nm. These findings offered a new clue for understanding the physicochemical properties of lattice dopants in lepidocrocite titanates.

General information
State: Published
Organisations: University of Oslo
Contributors: Gao, T., Fjellvåg, H., Norby, P.
Pages: 787-794
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry
Volume: 19
Issue number: 6
ISSN (Print): 0959-9428
Ratings:
Web of Science (2017): Indexed yes
BFI (2015): BFI-level 2
BFI (2014): BFI-level 2

Protonic titanate derived from CsxTi2-x/2Mgx/2O4 (x=0.7) with lepidocrocite-type layered structure
A layered titanate CsxTi2-x/2Mgx/2O4 (x = 0.7) with lepidocrocite (gamma-FeOOH)-type layered structure was prepared via solid-state reaction. Extraction of both Mg2+ ions in the host layers and interlayer Cs+ ions was achieved during an acid-exchange process, producing a new protonic titanate HxTi2-x/2O4-x/2 center dot H2O. This phase was distinguished from isomorphous related compounds in terms of removable lattice Mg and O atoms. The protonic titanate HxTi2-x/2O4-x/2 center dot H2O showed excellent exfoliation/delamination reactivity upon intercalating organic amine ions as well as the ability to produce single two-dimensional titanate nanosheets with small thickness of about 1 nm. These findings offered a new clue for understanding the physicochemical properties of lattice dopants in lepidocrocite titanates.
SAPO-34 methanol-to-olefin catalysts under working conditions: A combined in situ powder X-ray diffraction, mass spectrometry and Raman study

We have studied the behaviour of the zeotype silicoaluminophosphate SAPO-34 catalyst in the methanol-to-olefin (MTO) process under real working conditions using simultaneous synchrotron powder X-ray diffraction (PXRD) and Raman spectroscopy with online analysis of products by mass spectrometry. Anisotropic changes in the unit-cell dimensions are shown to be related to the build-up of intermediate species in the cages of the SAPO-34 framework and also to the deactivation of the catalyst (observed from the products in the mass spectra). We have quantified the amount of intermediate material in the cages from the PXRD using Fourier mapping techniques and our measurements are comparable with tapered element-oscillating microbalance measurements of coke build-up. Raman spectra indicate that the nature of the coke becomes increasingly graphitic with time. Our results also show that the catalyst recovers its original structural parameters when regenerated in air at 500-550 degrees C. (c) 2009 Elsevier Inc. All rights reserved.

General information
State: Published
Organisations: University of Oslo
Pages: 290-296
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Journal of Catalysis
Volume: 268
Issue number: 2
ISSN (Print): 0021-9517
Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.99 SJR 2.397 SNIP 1.85
Web of Science (2017): Impact factor 6.759
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.451 SNIP 2.142
Web of Science (2016): Impact factor 6.844
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 7.23 SJR 2.668 SNIP 2.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.92 SJR 2.688 SNIP 2.233
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.42 SJR 2.553 SNIP 2.091
Web of Science (2013): Impact factor 6.073
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.17 SJR 3.006 SNIP 2.257
Web of Science (2012): Impact factor 5.787
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.23 SJR 3.092 SNIP 2.214
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.38 SNIP 2.193
Web of Science (2010): Impact factor 5.415
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.965 SNIP 2.135
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.123 SNIP 2.164
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.15 SNIP 2.138
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.137 SNIP 2.043
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.99 SNIP 2.17
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.623 SNIP 2.015
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.407 SNIP 1.783
Structural and morphological evolution of beta-MnO₂ nanorods during hydrothermal synthesis

beta-MnO₂ nanorods were synthesized via a redox reaction of (NH₄)₂S₂O₈ and MnSO₄ under hydrothermal conditions. In situ and ex situ x-ray diffraction and scanning electron microscopy were employed to follow the structural and morphological evolution during growth. It was found that the crystallization of beta-MnO₂ nanorods proceeds through two steps: gamma-MnO₂ nanorods form first via a dissolution-recrystallization process and then transform topologically into beta-MnO₂ with increasing temperature. The phase transformation was associated with a short-range rearrangement of MnO₆ octahedra. Vibrational spectroscopic studies showed that the beta-MnO₂ nanorods had four infrared absorptions at 726, 552, 462 and 418 cm⁻¹ and four Raman scattering bands at 759 (B₂g), 662 (A₁g)), 576 (Ramsdellite impurity) and 537 (Eg) cm⁻¹, which are in agreement with Mn-O lattice vibrations within a rutile-type MnO₆ octahedral matrix.

General information
State: Published
Organisations: University of Oslo
Contributors: Gao, T., Fjellvåg, H., Norby, P.
Pages: 055610
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Nanotechnology
Volume: 20
Issue number: 5
ISSN (Print): 0957-4484
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.01 SJR 1.079 SNIP 0.788
Web of Science (2017): Impact factor 3.404
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.945
Web of Science (2016): Impact factor 3.44
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.07 SJR 1.257 SNIP 1.035
Web of Science (2015): Impact factor 3.573
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.09 SJR 1.497 SNIP 1.269
Web of Science (2014): Impact factor 3.821
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Syntheses, Structures, and Magnetic Properties of Nickel-Doped Lepidocrocite Titanates

Ni-doped titanate Cs_{x}Ti_{2−x/2}Ni_{x/2}O_{4} and its protonic derivative H_{x}Ti_{2−x/2}Ni_{x/2}O_{4}·xH_{2}O (x = 0.7) were synthesized and characterized by means of synchrotron X-ray diffraction, Raman scattering, X-ray photoelectron spectroscopy (XPS), and magnetic measurements. Cs_{x}Ti_{2−x}Ni_{x}O_{4} crystallizes in an orthorhombic structure (space group Immm), consisting of infinite two-dimensional (2D) host layers of the lepidocrocite (γ-FeOOH) type. The substitution of Ni atoms for Ti in the 2D octahedral layers results in negative charges that are compensated by interlayer Cs⁺ ions. Raman scattering and XPS indicate that local structural perturbations are induced upon exchange of interlayer Cs ions with protons H_{3}O⁺. Magnetic measurements reveal typical paramagnetism induced by Ni substitution; the effective paramagnetic moment μ_{eff} = 1.57(1) μB and Curie–Weiss temperature −2.51(1) K are obtained for H_{x}Ti_{2−x/2}Ni_{x/2}O_{4}·xH_{2}O. Ni- and Mg-codoped titanates
CsxTi2−x/2(NiyMg1−y)x/2O4 (x = 0.7, 0 ≤ y ≤ 1) were also reported. The crystal structure, interlayer chemistry, and magnetic properties of the titanates depend on the Ni substitution levels, indicating opportunities for tuning of the properties by controlling the nature and level of lattice substitutions.
Temperature dependant X-ray diffraction study of PrSr3Co1.5Fe1.5O10-d; n=3 Ruddlesden-Popper phase

The thermal evolution of the crystal structure of PrSr3Co1.5Fe1.5O10-d, a member of the n = 3 family of Ruddlesden-Popper compounds, has been studied by means of variable temperature synchrotron X-ray powder diffraction combined with room temperature neutron diffraction studies. This structure takes the ideal tetragonal I4/mmm (n = 139) space group. The possibility of symmetry lowering to the Pbca (n = 61) space group by slight tilting and rotation of the oxygen atoms around the octahedral B site is discussed. The non linear thermal expansion of the compound in air is caused by a chemical expansion accompanying the loss of oxygen that comes in addition to normal thermal expansion. A mechanism describing the creation of oxygen vacancies is proposed.

General information
State: Published
Organisations: University of Oslo, University of Liverpool
Contributors: Jantsky, L., Norby, P., Rosseinsky, M. J., Fjellvåg, H.
Pages: 295-301
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Zeitschrift für Kristallographie - Crystalline Materials
Volume: 224
Issue number: 5-6
ISSN (Print): 2194-4946
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.95 SJR 2.139 SNIP 5.371
Web of Science (2017): Impact factor 1.263
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.54 SJR 1.067 SNIP 2.883
Web of Science (2016): Impact factor 3.179
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.33 SJR 0.803 SNIP 1.291
Web of Science (2015): Impact factor 2.56
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.21 SJR 0.589 SNIP 0.753
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.25 SJR 0.644 SNIP 0.796
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.15 SJR 0.611 SNIP 0.825
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.13 SJR 0.671 SNIP 0.767
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.079 SNIP 0.899
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.993 SNIP 0.752
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.96 SNIP 1.076
Scopus rating (2007): SJR 0.91 SNIP 1.01
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.948 SNIP 1.202
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.525 SNIP 0.792
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.466 SNIP 0.918
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.411 SNIP 0.751
Scopus rating (2002): SJR 0.609 SNIP 0.848
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.542 SNIP 0.942
Scopus rating (2000): SJR 0.495 SNIP 1.163
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.527 SNIP 0.74
Original language: English
DOI:
10.1524/zkri.2009.1156
Source: orbit
Source-ID: 256922
Research output: Research - peer-review › Journal article – Annual report year: 2009

Projects:

**Graphene supported transition metal oxide composites as metal-ion battery electrode materials**
cao, H., PhD Student, Department of Chemistry
Chi, Q., Main Supervisor, Department of Chemistry
Mossin, S., Supervisor, Department of Chemistry
Norby, P., Supervisor
Stipendie fra udlandet
01/01/2018 → 31/12/2020
Award relations: Graphene supported transition metal oxide composites as metal-ion battery electrode materials
Project: PhD

**Next generation rechargeable batteries: Sustainable and earth-abundant materials**
Christensen, M. K., PhD Student, Department of Energy Conversion and Storage
Norby, P., Main Supervisor, Department of Energy Conversion and Storage
Hoster, H. E., Supervisor
Vegge, T., Supervisor, Department of Energy Conversion and Storage
Samfinansieret - Andet
01/12/2015 → 30/11/2018
Award relations: Next generation rechargeable batteries: Sustainable and earth-abundant materials
Project: PhD

**Development and characterization of emerging battery electrodes and electrolytes**
Lefevr, J., PhD Student, Department of Energy Conversion and Storage
Blanchard, D., Main Supervisor, Department of Energy Conversion and Storage
Hoster, H. E., Supervisor
Norby, P., Supervisor, Department of Energy Conversion and Storage
Institut stipendie (DTU)
01/12/2015 → 30/11/2018
Award relations: Development and characterization of emerging battery electrodes and electrolytes
Project: PhD

**Green Production of Nanomaterials for Energy Conversion**
Xu, Y., PhD Student, Department of Energy Conversion and Storage
Kiebach, W., Main Supervisor, Department of Energy Conversion and Storage
Hendriksen, P. V., Supervisor, Department of Energy Conversion and Storage
Norby, P., Supervisor, Department of Energy Conversion and Storage
Simonsen, S. B., Supervisor, Department of Energy Conversion and Storage
Della Negra, M., Examiner, Department of Energy Conversion and Storage
Aymonier, C., Examiner
Lester, E. H., Examiner
Forskningsrådsfinansiering
01/07/2014 → 30/09/2017
Award relations: Green Production of Nanomaterials for Energy Conversion
Project: PhD

**Electrochemical Reduction of CO2 to Sustainable Synthetic Fuels**
Bhowmik, A., PhD Student, Department of Energy Conversion and Storage
Vegge, T., Main Supervisor, Department of Energy Conversion and Storage
Hansen, H. A., Supervisor, Department of Energy Conversion and Storage
Norby, P., Examiner, Department of Energy Conversion and Storage
Skulason, E., Examiner
Studt, F., Examiner
Samfinansieret - Andet
01/06/2014 → 20/09/2017
Award relations: Electrochemical Reduction of CO2 to Sustainable Synthetic Fuels
Project: PhD

**In situ characterisation of structure and transport in battery electrolytes and electrodes**
Sveinbjörnsson, D. P., PhD Student, Department of Energy Conversion and Storage
Vegge, T., Main Supervisor, Department of Energy Conversion and Storage
Mogensen, M. B., Supervisor, Department of Energy Conversion and Storage
Norby, P., Supervisor, Department of Energy Conversion and Storage
Hjelm, J., Examiner, Department of Energy Conversion and Storage
David, W. I. F., Examiner
Serby, M. H., Examiner
Globaliseringsmidler
01/01/2011 → 26/02/2014
Award relations: In situ characterisation of structure and transport in battery electrolytes and electrodes
Project: PhD

Dynamical properties of nano-structured catalysts for methane conversion
Kehres, J., PhD Student, Risø National Laboratory for Sustainable Energy
Vegge, T., Main Supervisor, Risø National Laboratory for Sustainable Energy
Andreasen, J. W., Supervisor, Risø National Laboratory for Sustainable Energy
Chorkendorff, I., Supervisor, Risø National Laboratory for Sustainable Energy
Molenbrock, A., Supervisor
Norby, P., Examiner, Risø National Laboratory for Sustainable Energy
Bouwman, W., Examiner
Grunwaldt, J., Examiner
1/3 FU, 1/3 inst 1/3 Andet
01/09/2007 → 20/04/2011
Award relations: Dynamical properties of nano-structured catalysts for methane conversion
Project: PhD

Preparation and characterization of cathode materials for lithium-oxygen batteries
Storm, M. M., PhD Student, Department of Energy Conversion and Storage
Norby, P., Main Supervisor, Department of Energy Conversion and Storage
Luntz, A., Supervisor
Blanchard, D., Examiner, Department of Energy Conversion and Storage
Choi, J. W., Examiner
Nørgaard, K., Examiner
Forskningsrådsfinansiering
15/08/2012 → 20/09/2016
Award relations: Preparation and characterization of cathode materials for lithium-oxygen batteries
Project: PhD

Management of Lithium-air batteries - safety, reliability and performance
Christensen, A. E., PhD Student, Department of Energy Conversion and Storage
Norby, P., Main Supervisor, Department of Energy Conversion and Storage
Larsen, E., Supervisor
Vestin, K., Supervisor
Jensen, S. H., Examiner, Department of Energy Conversion and Storage
Monroe, C. W., Examiner
Møller, P. J., Examiner
Forskningsrådsstipendium
01/12/2012 → 20/04/2016
Award relations: Management of Lithium-air batteries - safety, reliability and performance
Project: PhD

Development of novel electrode-catalyst materials for Li-air battery cathodes
Højberg, J., PhD Student, Department of Energy Conversion and Storage
Vegge, T., Main Supervisor, Department of Energy Conversion and Storage
Johansen, K., Supervisor
Norby, P., Supervisor, Department of Energy Conversion and Storage
García Lastra, J. M., Examiner, Department of Energy Conversion and Storage
Edström, E. K., Examiner
Hoster, H. E., Examiner
Forskningsrådsstipendium
01/01/2012 → 01/07/2015
Award relations: Development of novel electrode-catalyst materials for Li-air battery cathodes
Project: PhD

Performance and lifetime limiting effects in Li-ion batteries
Scipioni, R., PhD Student, Department of Energy Conversion and Storage
Jensen, S. H., Main Supervisor, Department of Energy Conversion and Storage
Hjelm, J., Supervisor, Department of Energy Conversion and Storage
Norby, P., Supervisor, Department of Energy Conversion and Storage
Bowen, J. R., Examiner, Department of Energy Conversion and Storage
Bowen, J. R., Examiner, Department of Energy Conversion and Storage
Lindbergh, G., Examiner
Lindbergh, G., Examiner
Offentlig finansiering
01/06/2013 → 20/09/2016
Award relations: Performance and lifetime limiting effects in Li-ion batteries
Project: PhD

**Udvikling og karakterisering af avancerede Li-batterier**
Christiansen, A. S., PhD Student, Department of Energy Conversion and Storage
Holtappels, P., Main Supervisor, Department of Energy Conversion and Storage
Jensen, S. H., Supervisor, Department of Energy Conversion and Storage
Norby, P., Supervisor, Department of Energy Conversion and Storage
Pedersen, A. S., Examiner, Department of Energy Conversion and Storage
Dahl, S., Examiner
Dominko, R., Examiner
Institut, samfinansiering
01/03/2011 → 02/09/2015
Award relations: Udvikling og karakterisering af avancerede Li-batterier
Project: PhD

**In-situ TEM Studies of Nanowire-based Batteries**
Møller-Nilsen, R. E. R., PhD Student, Department of Micro- and Nanotechnology
Mølhave, K., Main Supervisor, Department of Micro- and Nanotechnology
Norby, P., Supervisor
Wagner, J. B., Supervisor
Booth, T., Examiner, Department of Micro- and Nanotechnology
Alloyeau, D., Examiner
Tang, P. T., Examiner
Institut, samfinansiering
15/12/2012 → 15/06/2016
Award relations: In-situ TEM Studies of Nanowire-based Batteries
Project: PhD

**High Performance polymer solar cells through rational characterization and design**
Tromholt, T., PhD Student, Department of Energy Conversion and Storage
Krebs, F. C., Main Supervisor, Department of Energy Conversion and Storage
Norby, P., Examiner, Department of Energy Conversion and Storage
Nelson, J., Examiner
Rivaton, A., Examiner
Forskningsrådsfinansiering
01/07/2009 → 19/10/2012
Award relations: High Performance polymer solar cells through rational characterization and design
Project: PhD

**Activities:**

**Lithium batterier til transport. Er det vejen frem?**
Period: 23 Sep 2010
Poul Norby (Speaker)
Risø National Laboratory for Sustainable Energy
Materials Research Division
Nano-Microstructures in Materials

**Description**
Place: Elektronikmessen, Odense (DK)

**Related external organisation**

Unknown external organisation
Activity: Talks and presentations › Conference presentations
In situ studies of lithium batteries using high energy synchrotron X-ray diffraction
Period: 8 Sep 2010
Poul Norby (Speaker)
Risø National Laboratory for Sustainable Energy
Materials Research Division
Nano-Microstructures in Materials

Related event
High-Energy X-Ray Beamlines at the PETRA III Extension Workshop
08/09/2010 → …
Hamburg, Germany
Activity: Talks and presentations › Conference presentations

In situ diffraction studies of materials for energy technology
Period: 6 May 2010
Poul Norby (Lecturer)
Materials Research Division
Nano-Microstructures in Materials
Risø National Laboratory for Sustainable Energy

Related external organisation
IMFUFA course, Roskilde (DK)
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities