Diluted Oxide Interfaces with Tunable Ground States

The metallic interface between two oxide insulators, such as LaAlO3/SrTiO3 (LAO/STO), provides new opportunities for electronics and spintronics. However, due to the presence of multiple orbital populations, tailoring the interfacial properties such as the ground state and metal-insulator transitions remains challenging. Here, we report an unforeseen tunability of the phase diagram of LAO/STO by alloying LAO with a ferromagnetic LaMnO3 insulator without forming lattice disorder and at the same time without changing the polarity of the system. By increasing the Mn-doping level, x, of LaAl1-xMnx O3/STO (0 ≤ x ≤ 1), the interface undergoes a Lifshitz transition at x = 0.225 across a critical carrier density of nc = 2.8×10¹³ cm⁻², where a peak TSC = 255 mK of superconducting transition temperature is observed. Moreover, the LaAl1-xMnxO3 turns ferromagnetic at x ≥ 0.25. Remarkably, at x = 0.3, where the metallic interface is populated by only dxy electrons and just before it becomes insulating, we achieve reproducibly a same device with both signatures of superconductivity and clear anomalous Hall effect (7.6×10¹² cm⁻² < ns ≤ 1.1×10¹³ cm⁻²). This provides a unique and effective way to tailor oxide interfaces for designing on-demand electronic and spintronic devices.
The role of oxide interfaces in highly confined electronic and ionic conductors

Oxides bring not only new properties such as superconductivity, ferro-, pyro-, and piezoelectricity, ferromagnetism, and multiferroicity but also ionic and catalytic properties. Such richness arises from a strong interaction between the charge, orbital, spin, and lattice degrees of freedom. Interfacing two oxide-based materials results in broken lattice symmetry as well as electronic and/or atomic reconstructions from which a wealth of new intriguing properties can emerge. Here, we provide an overview and perspective of electronic, ionic, and ionotronic properties in oxide systems with confinement designed by broken lattice symmetry.

General information
Tuning the stoichiometry and electrical properties of tantalum oxide thin films

Tantalum oxide has a wide range of applications and has drawn much attention especially for its useful properties in resistive random-access memories, in which the Ta oxide composition plays an important role to control the electrical properties of the TaOx thin films. In this paper, we present a way to tune the composition of TaOx thin films by varying the oxygen partial pressure during growth using pulsed laser deposition. TaOx thin films were deposited at room temperature, under oxygen partial pressures ranging from 10^-6 mbar to 2*10^-2 mbar. Using angle resolved X-ray photoelectron spectroscopy, we show that the composition of the film varies systematically with the oxygen partial pressure during the film growth. We then correlate the oxygen content with the electrical properties of the film and the results show that the composition has a great influence on the resistivity of the TaOx thin films. As the oxygen partial pressure during deposition increases, the percentage of tantalum pentoxide (Ta2O5) as well as the resistivity of the films increases. This experimental approach provides a pathway to control the TaOx thin film stoichiometry and its electrical properties during growth.
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
Web of Science (2013): Impact factor 2.538
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.26 SJR 0.913 SNIP 1.362
Web of Science (2012): Impact factor 2.112
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.922 SNIP 1.126
Web of Science (2010): Impact factor 1.795
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.84 SNIP 1.024
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.89 SNIP 1.084
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.791 SNIP 0.935
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.861 SNIP 1.046
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.689 SNIP 0.938
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.984 SNIP 1.123
Scopus rating (2003): SJR 1.017 SNIP 1.036
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.954 SNIP 0.97
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.874 SNIP 0.804
2D hole gas seen
A p-type metallic sheet forms between two oxide insulators, LaAlO3 and SrTiO3. Suppression of oxygen vacancies in SrTiO3 plays a critical role in forming this sheet.
Direct Demonstration of the Emergent Magnetism Resulting from the Multivalence Mn in a LaMnO3 Epitaxial Thin Film System

Atomically engineered oxide heterostructures provide a fertile ground for creating novel states, for example, a 2D electron gas at the interface between two oxide insulators, giant thermoelectric Seebeck coefficient, emergent ferromagnetism from otherwise nonmagnetic components, and colossal ionic conductivity. Extensive research efforts reveal that oxygen deficiency or lattice strain play an important role in determining these unexpected properties. Herein, by studying the abrupt presence of robust ferromagnetism (up to 1.5 µB/Mn) in LaMnO3-based heterostructures, the multivalence states of Mn that play a decisive role in the emergence of ferromagnetism in the otherwise antiferromagnetic LaMnO3 thin films are found. Combining spatially resolved electron energy-loss spectroscopy, X-ray absorption spectroscopy, and X-ray magnetic circular dichroism techniques, it is determined unambiguously that the ferromagnetism results from a conventional Mn3+-O–Mn4+ double-exchange mechanism rather than an interfacial effect. In contrast, the magnetic dead layer of 5 unit cell in proximity to the interface is found to be accompanied with the accumulation of Mn2+ induced by electronic reconstruction. These findings provide a hitherto-unexplored multivalence state of Mn on the emergent magnetism in undoped manganite epitaxial thin films, such as LaMnO3 and BiMnO3, and shed new light on all-oxide spintronic devices.

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Article number: 1800055
Ratings:
Web of Science (2018): Indexed yes
Effects of accelerated degradation on metal supported thin film-based solid oxide fuel cell

A thin film-based solid oxide fuel cell is deposited on a Ni-based metal porous support by pulsed laser deposition with a multi-scale-graded microstructure design. The fuel cell, around 1 μm in thickness, is composed of a stabilized-zirconia/doped-ceria bi-layered dense electrolyte and nanostructured Ni-stabilized zirconia and La$_{0.6}$Sr$_{0.4}$CoO$_3$ electrodes as the anode and cathode, respectively. The cell is tested at intermediate temperatures (600–650 °C) with the aim to discern the degradation mechanisms occurring in the cell under accelerated conditions. Under open circuit conditions, electrochemical performances are steady, indicating the stability of the cell. Under electrical load, a progressive degradation is activated. Post-test analysis reveals both mechanical and chemical degradation of the cell. Cracks and delamination of the thin films promote a significant nickel diffusion and new phase formation. Signs of elemental distribution at low temperature are detected throughout the cell, indicating a combination of low energy surface elemental interdiffusion and electromigration effects.

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Contributors: Reolon, R. P., Sanna, S., Xu, Y., Lee, I., Bergmann, C. P., Pryds, N., Esposito, V.
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
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
Electron mobility in oxide heterostructures: Topical review

Next-generation integrated circuit devices based on transition-metal-oxides are expected to boast a variety of extraordinary properties, such as superconductivity, transparency in the visible range, thermoelectricity, giant ionic conductivity and ferromagnetism. However, the realisation of this so-called oxide electronics as well as the study of their unconventional physics is stalled by inferior carrier mobilities compared to conventional semiconductor materials. Over the past 10 years, bulk conducting oxides and oxide heterostructures with superior carrier mobilities have nonetheless seen significant progress. This progress is signifying the approaching era of oxide-based electronic circuits along with novel solid-state phenomena originating from the combination of hybridized oxygen p orbitals, transition-metal d orbitals and electronic correlations. Here, we review the recent advancements and results on high mobility oxide heterostructures based on SrTiO3 and ZnO as well as other prominent oxides.
Electron Mobility in γ-Al₂O₃/SrTiO₃

One of the key issues in engineering oxide interfaces for electronic devices is achieving high electron mobility. SrTiO₃-based interfaces with high electron mobility have gained a lot of interest due to the possibility of combining quantum phenomena with the many functionalities exhibited by SrTiO₃. To date, the highest electron mobility (140 000 cm²/V s at 2 K) is obtained by interfacing perovskite SrTiO₃ with spinel γ-Al₂O₃. The origin of the high mobility, however, remains poorly understood. Here, we investigate the scattering mechanisms limiting the mobility in γ-Al₂O₃/SrTiO₃ at temperatures between 2 and 300 K and over a wide range of sheet carrier densities. For T>150 K, we find that the mobility is limited by longitudinal optical phonon scattering. For large sheet carrier densities (>8×10¹³ cm⁻²), the screened electron-phonon coupling leads to room-temperature mobilities up to μ∼12 cm²/V s. For 5 K...

Emergent ferromagnetism in an otherwise antiferromagnetic LaMnO3-based heterostructure attributable to the cation-vacancy-induced oxygen excess effect through direct observation of multivalence Mn is reported by Xuefeng Wang, Peng Wang, Yongbing Xu, Yunzhong Chen, and co-workers in article number 1800055. The ferromagnetism is mediated by the Mn3+-O–Mn4+ double-exchange mechanism. It provides a hitherto unexplored multivalence state of Mn on the emergent ferromagnetism in manganite thin films.
Enhanced visible light catalytic activity of MoS2/TiO2/Ti photocathode by hybrid-junction

In photoelectrochemical (PEC) water splitting systems, crucial obstacles limiting their performance are poor charge carrier dynamics and high recombination rate of photoexcited electron hole pairs. Here, we report that this issue can be alleviated by engineering a hybrid-junction that is composed of homo- and hetero-junctions. This strategy is performed by facile hand-spraying MoS2 over the surface of a anatase/rutile homo-junction TiO2 film on the Ti substrate to further form a hybrid-junction photocathode. By applying this photocathode into PEC reactor, enhanced catalytic activity is achieved under visible light (AM1.5 illumination of 300W/m2) with hydrogen evolution reaction (HER) potential of −114mV versus reversible hydrogen electrode (RHE) at 10mA/cm2 and long-term stability of more than 10 times improvement comparing to ordinary electrode without the introduction of hybrid-junction. The hybrid-junction that effectively regulates charge separation and transfer pathways is proven to be responsible for the enhanced activity. As an novel exploration, this hybrid-junction system comprising of low-cost, efficient charge separation and transfer, and visible light responsivity offers a new path for relative materials to boost their PEC performance.

General information
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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 10.92 SJR 3.152 SNIP 2.359
Web of Science (2017): Impact factor 11.698
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.693 SNIP 2.185
Web of Science (2016): Impact factor 9.446
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 7.72 SJR 2.326 SNIP 2.16
Web of Science (2015): Impact factor 8.328
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.92 SJR 2.322 SNIP 2.206
Web of Science (2014): Impact factor 7.435
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.42 SJR 2.391 SNIP 2.154
Web of Science (2013): Impact factor 6.007
ISI indexed (2013): ISI indexed yes
Extreme Reconfigurable Nanoelectronics at the CaZrO$_3$/SrTiO$_3$ Interface

Complex oxide heterostructures have fascinating emergent properties that originate from the properties of the bulk constituents as well as from dimensional confinement. The conductive behavior of the polar/nonpolar LaAlO$_3$/SrTiO$_3$ interface can be reversibly switched using conductive atomic force microscopy (c-AFM) lithography, enabling a wide range of devices and physics to be explored. Here, extreme nanoscale control over the CaZrO$_3$/SrTiO$_3$ (CZO/STO) interface, which is formed from two materials that are both nonpolar, is reported. Nanowires with measured widths as narrow as 1.2 nm are realized at the CZO/STO interface at room temperature by c-AFM lithography. These ultrathin nanostructures have spatial dimensions at room temperature that are comparable to single-walled carbon nanotubes, and hold great promise for alternative oxide-based nanoelectronics, as well as offer new opportunities to investigate the electronic structure of the complex oxide interfaces. The cryogenic properties of devices constructed from quasi-1D channels, tunnel barriers, and planar gates exhibit gate-tunable superconductivity, quantum oscillations, electron pairing outside of the superconducting regime, and quasi-ballistic transport. This newly demonstrated ability to control the metal-insulator transition at nonpolar oxide interface greatly expands the class of materials whose behavior can be patterned and reconfigured at extreme nanoscale dimensions.
High-temperature thermoelectric properties of Na- and W-Doped Ca$_3$Co$_4$O$_9$ system

The detailed crystal structures and high temperature thermoelectric properties of polycrystalline Ca$_{3-2x}$Na$_{2x}$Co$_{4-x}$W$_x$O$_9$ ($0 \leq x \leq 0.075$) samples have been investigated. Powder X-ray diffraction data show that all samples are phase pure, with no detectable traces of impurity. The diffraction peaks shift to lower angle values with increase in doping ($x$), which is consistent with larger ionic radii of Na$^+$ and W$^{6+}$ ions. X-ray photoelectron spectroscopy data reveal that a mixture of Co$^{2+}$, Co$^{3+}$ and Co$^{4+}$ valence states are present in all samples. It has been observed that electrical resistivity ($\rho$), Seebeck coefficient ($S$) and thermal conductivity ($\kappa$) are all improved with dual doping of Na and W in Ca$_3$Co$_4$O$_9$ system. A maximum power factor (PF) of $2.71 \times 10^{-4}$ W m$^{-1}$ K$^{-2}$ has been obtained for $x = 0.025$ sample at 1000 K. The corresponding thermoelectric figure of merit ($zT$) for $x = 0.025$ sample is calculated to be 0.21 at 1000 K, which is $\approx 2.3$ times higher than $zT$ value of the undoped sample. These results suggest that Na and W dual doping is a promising approach for improving thermoelectric properties of Ca$_3$Co$_4$O$_9$ system.

General information
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736
Web of Science (2017): Impact factor 2.936
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Web of Science (2016): Impact factor 3.108
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834
Web of Science (2015): Impact factor 3.289
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.87 SJR 1.113 SNIP 0.962
Web of Science (2014): Impact factor 3.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.74 SJR 1.119 SNIP 0.904
Nanoscale patterning of electronic devices at the amorphous LaAlO3/SrTiO3 oxide interface using an electron sensitive polymer mask

A simple approach is presented for designing complex oxide mesoscopic electronic devices based on the conducting interfaces of room temperature grown LaAlO3/SrTiO3 heterostructures. The technique is based entirely on methods known from conventional semiconductor processing technology, and we demonstrate a lateral resolution of similar to 100 nm. We study the low temperature transport properties of nanoscale wires and demonstrate the feasibility of the technique for defining in-plane gates allowing local control of the electrostatic environment in mesoscopic devices. (C) 2018 Author(s).
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Impact factor 3.495
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Impact factor 3.411
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.47 SJR 1.499 SNIP 1.226
Web of Science (2015): Impact factor 3.142
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.25 SJR 1.861 SNIP 1.492
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.77 SJR 2.146 SNIP 1.633
Web of Science (2013): Impact factor 3.515
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.76 SJR 2.57 SNIP 1.739
Web of Science (2012): Impact factor 3.794
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.04 SJR 2.814 SNIP 1.917
Web of Science (2011): Impact factor 3.844
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Impact factor 3.841
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.012 SNIP 1.916
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.755 SNIP 2.353
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.992 SNIP 2.367
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.897 SNIP 2.275
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 4.018 SNIP 2.414
Near interface ionic transport in oxygen vacancy stabilized cubic zirconium oxide thin films

The cubic phase of pure zirconia (ZrO₂) is stabilized in dense thin films through a controlled introduction of oxygen vacancies (O defects) by cold-plasma-based sputtering deposition. Here, we show that the cubic crystals present at the film/substrate interface near-region exhibit fast ionic transport, which is superior to what is obtained with similar yttrium-stabilized cubic zirconia thin films.

General information

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Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Ceramic Engineering & Science, University of Mons, University of Málaga, Université de Nantes
Contributors: Raza, M., Sanna, S., Dos Santos Gómez, L., Gautron, E., El Mel, A. A., Pryds, N., Snyders, R., Konstantinidis, S., Esposito, V.
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
Strain-tunable magnetism at ferroelastic domain walls

Applying stress to a ferroelastic material results in a nonlinear strain response as domains of different orientations mechanically switch. The ability to write, erase and move domain walls between such ferroelastic domains suggests a method for making nanoelectronics where the domain wall is the device. However, little is known about the magnetic properties of such domain walls. A fascinating model system is SrTiO$_3$, where the ferroelastic domain walls display strain-tunable polarity and enhanced conductivity. Here, we reveal a long-range magnetic order with modulations along the ferroelastic domain walls in SrTiO$_3$ and SrTiO$_3$-based heterointerfaces, which manifests itself as a striped pattern in scanning superconducting quantum interference device maps of the magnetic landscape. In conducting interfaces, the magnetism is coupled to itinerant electrons with clear signatures in magnetotransport measurements. The magnetic state is also coupled dynamically to the lattice and can be reversibly tuned by applying local external forces. This study raises the possibility of designing nanoscale devices based on domain walls where strain-tunable ferroelectric, ferroelastic and ferromagnetic orders may coexist.
Tuning the Ground State of Oxide Interfaces by an Electron Sink

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

Chemical redox reaction can lead to a two-dimensional electron gas (2DEG) at the interface between a TiO2-terminated SrTiO3 (STO) substrate and an amorphous LaAlO3 (a-LAO) capping layer. When replacing the STO substrate with rutile and anatase TiO2 substrates, considerable differences in interfacial conduction are observed. Based on X-ray photoelectron spectroscopy (XPS) and transport measurements, we conclude that the interfacial conduction comes from redox reactions, and that the differences among the materials systems result mainly from variations in the activation energies for the diffusion of oxygen vacancies at substrate surfaces.

**General information**

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences, Technical University of Denmark
A regenerative elastocaloric device: Experimental results

Elastocaloric cooling and heating is an alternative cooling technology that has potential to be highly efficient and environmentally friendly. Experimental results are reported for two elastocaloric regenerators made of NiTi alloys in the form of parallel plates in two plate thicknesses. For the regenerator made of 0.2 mm plates, a maximum no-load temperature span of 17.6 K was achieved for an applied strain of 4.3 %. For the regenerator with 0.35 mm plates, a maximum temperature span of 19.9 K was reached for a strain of 3.5 %. The 0.2 mm regenerator failed after approximately 5200 cycles and the 0.35 mm regenerator failed after approximately 5500 cycles.

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BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Impact factor 2.373
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Impact factor 2.588
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.1 SJR 0.886 SNIP 1.25
Web of Science (2015): Impact factor 2.772
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.53 SJR 1.096 SNIP 1.408
Web of Science (2014): Impact factor 2.721
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.6 SJR 1.194 SNIP 1.452
Web of Science (2013): Impact factor 2.521
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.31 SJR 1.279 SNIP 1.414
Web of Science (2012): Impact factor 2.528
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.36 SJR 1.266 SNIP 1.399
Web of Science (2011): Impact factor 2.544
ISI indexed (2011): ISI indexed yes
Controlling the Carrier Density of SrTiO₃-Based Heterostructures with Annealing

The conducting interface between the insulating oxides LaAlO₃ (LAO) and SrTiO₃ (STO) displays numerous physical phenomena that can be tuned by varying the carrier density, which is generally achieved by electrostatic gating or adjustment of growth parameters. Here, it is reported how annealing in oxygen at low temperatures (T < 300 °C) can be used as a simple route to control the carrier density by several orders of magnitude. The pathway to control the carrier density relies on donor oxidation and is thus applicable to material systems where oxygen vacancies are the dominant source of conductivity. Using STO capped with epitaxial γ-Al₂O₃ (GAO) or amorphous LAO (a-LAO), the pathways for changing the carrier density in the two STO-based cases are identified where oxygen blocking (GAO) and oxygen permeable (a-LAO) films create interface conductivity from oxygen vacancies located near the interface. For a-LAO/STO, the rate limiting step (Eₐ = 0.25 eV) for oxidizing oxygen vacancies is the transportation of oxygen from the atmosphere through the a-LAO film, whereas GAO/STO is limited by oxygen migration inside STO (Eₐ = 0.5 eV). Finally, it is shown how the control of the carrier density enables writing of conducting nanostructures in γ-Al₂O₃/STO by conducting atomic force microscopy.
Effect of Sr-doping of LaMnO$_3$ spacer on modulation-doped two-dimensional electron gases at oxide interfaces

Modulation-doped oxide two-dimensional electron gas formed at the LaMnO$_3$ (LMO) buffered disordered-LaAlO$_3$/SrTiO$_3$ (d-LAO/LMO/STO) heterointerface provides new opportunities for electronics as well as quantum physics. Herein, we studied the dependence of Sr-doping of La$_{1-x}$Sr$_x$MnO$_3$ (LSMO, x = 0, 1/8, 1/3, ½, and 1) spacer on the transport properties of d-LAO/LSMO/STO in order to determine the effects of the filling of Mn $e_g$ subbands as well as the LSMO polarity on the modulation-doping. Upon increasing the LSMO film thickness from 1 unit cell (uc) to 2 uc, a sharp metal to insulator transition of interface conduction was observed, independent of x. The resultant electron mobility is higher than 1900 cm$^2$ V$^{-1}$ s$^{-1}$ at 2K, which increases upon decreasing x. The sheet carrier density, on the other hand, is in the range of 6.9×10$^{12}$–1.8×10$^{13}$ cm$^{-2}$ (0.01–0.03 e/uc) and is largely independent on x for all the metallic d-LAO/LSMO (1 uc)/STO interfaces. These results are consistent with the charge transfer induced modulation doping scheme and clarify that the polarity of the buffer layer plays a trivial role on the modulation doping. The negligible tunability of the carrier density could result from the reduction of LSMO during the deposition of disordered LAO or that the energy levels of Mn 3$d$ electrons at the interface of LSMO/STO are hardly varied even when changing the LSMO composition from LMO to SrMnO$_3$.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Contributors: Chen, Y., Gan, Y., Christensen, D. V., Zhang, Y., Pryds, N.
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Efficient p-n junction-based thermoelectric generator that can operate at extreme temperature conditions

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

General information
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Impact factor 2.373
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Impact factor 2.588
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.1 SJR 0.886 SNIP 1.25
Web of Science (2015): Impact factor 2.772
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.53 SJR 1.096 SNIP 1.408
Web of Science (2014): Impact factor 2.721
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.6 SJR 1.194 SNIP 1.452
Web of Science (2013): Impact factor 2.521
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.31 SJR 1.279 SNIP 1.414
Web of Science (2012): Impact factor 2.528
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.36 SJR 1.266 SNIP 1.399
Web of Science (2011): Impact factor 2.544
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.292 SNIP 1.28
Web of Science (2010): Impact factor 2.109
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.269 SNIP 1.327
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.427 SNIP 1.549
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.38 SNIP 1.612
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.406 SNIP 1.742
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.216 SNIP 1.455
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.133 SNIP 1.438
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.912 SNIP 1.221
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.033 SNIP 1.233
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.925 SNIP 1.212
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.842 SNIP 1.125
Web of Science (2000): Indexed yes
Experimental Determination of the Formation Enthalpy of Calcium Cobaltate from Sol–Gel Precursors

Calcium cobaltate (Ca$_3$Co$_4$O$_9$) remains one of the most promising p-type oxide materials for high-temperature thermoelectric energy conversion. While much progress has been made in refining our understanding of the unique structure of the material, as well as optimization of the transport properties for thermoelectric efficiency, there remains a gap in the knowledge, both experimental and theoretical, of the thermodynamics of the system. Presented herein is an analysis of the heat of formation of the Ca$_3$Co$_4$O$_9$ phase from sol–gel precursors using a highly sensitive differential scanning calorimeter, as well as observations of its decomposition into the Ca$_3$Co$_2$O$_6$ phase. The reaction enthalpy of forming Ca$_3$Co$_4$O$_9$ from CaCO$_3$ and Co$_3$O$_4$ sol–gel precursors was determined to be +284 (±2%) kJ/mol, leading to a standard enthalpy of Ca$_3$Co$_4$O$_9$ of −3307 (±3.5%) kJ/mol.

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Scopus rating (2017): CiteScore 1.59 SJR 0.474 SNIP 0.772
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.754
Web of Science (2016): Impact factor 1.579
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.53 SJR 0.555 SNIP 0.802
Web of Science (2015): Impact factor 1.491
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.82 SJR 0.679 SNIP 1.05
Web of Science (2014): Impact factor 1.798
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.71 SJR 0.71 SNIP 1.094
Web of Science (2013): Impact factor 1.675
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Giant Electrostriction in highly defective oxides: The next generation of electromechanical materials.

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Contributors: Santucci, S., Esposito, V., Pryds, N.
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Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Giant tunability of the two-dimensional electron gas at the interface of γ-Al₂O₃/SrTiO₃
Two-dimensional electron gases (2DEGs) formed at the interface between two oxide insulators provide a rich platform for the next generation of electronic devices. However, their high carrier density makes it rather challenging to control the interface properties under a low electric field through a dielectric solid insulator, i.e. in the configuration of conventional field-effect transistors. To surpass this long-standing limit, we used ionic liquids as the dielectric layer for electrostatic gating of oxide interfaces in an electric double layer transistor (EDLT) configuration. Herein, we reported giant tunability of the physical properties of 2DEGs at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃(GAO/STO). By modulating the
carrier density thus the band filling with ionic-liquid gating, the system experiences a Lifshitz transition at a critical carrier
density of \(3.0 \times 10^{13} \text{ cm}^{-2}\), where a remarkably strong enhancement of Rashba spin-orbit interaction and an emergence of
Kondo effect at low temperatures are observed. Moreover, as the carrier concentration depletes with decreasing gating
voltage, the electron mobility is enhanced by more than 6 times in magnitude, leading to the observation of clear quantum
oscillations. The great tunability of GAO/STO interface by EDLT gating not only shows promise for design of oxide devices
with on-demand properties, but also sheds new light on the electronic structure of 2DEG at the non-isostructural
spinel/perovskite interface.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Chemistry,
Organic Chemistry, Technical University of Denmark, Nanjing University
Contributors: Niu, W., Zhang, Y., Gan, Y., Christensen, D. V., von Soosten, M., Garcia Suárez, E. J., Riisager, A., Wang,
X., Xu, Y., Zhang, R., Pryds, N., Chen, Y.
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BFI (2017): BFI-level 2
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
Web of Science (2011): Impact factor 13.198
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
In operando study of high-performance thermoelectric materials for power generation: a case study of $\beta$-Zn$_4$Sb$_3$

To bring current thermoelectric (TE) materials achievement into a device for power generation, a full understanding of their dynamic behavior under operating conditions is needed. Here, an in operando study is conducted on the high-performance TE material $\beta$-Zn$_4$Sb$_3$ under large temperature gradient and thermal cycling via a new approach using in situ transmission electron microscopy combined with characterization of the TE properties. It is found that after 30 thermal cycles in a low-pressure helium atmosphere the TE performance of $\beta$-Zn$_4$Sb$_3$ is maintained with the figure of merit, $zT$, value of 1.4 at 718 K. Under a temperature gradient of 380 K ($T_{\text{hot}} = 673$ K and $T_{\text{cold}} = 293$ K) operating for only 30 h, zinc whiskers gradually precipitate on the cold side of the $\beta$-Zn$_4$Sb$_3$ leg. The dynamical evolution of Zn in the matrix of $\beta$-Zn$_4$Sb$_3$ is found to be the source that leads to a high $zT$ value by lowering of the thermal conductivity and electrical resistivity, but it is also the failure mechanism for the leg under these conditions. The in operando study brings deep insight into the dynamic behavior of nanostructured TE materials for tailoring future TE materials and devices with higher efficiency and longer durability.
Magnetic two-dimensional electron gas at the manganite-buffered LaAlO$_3$/SrTiO$_3$ interface

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

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

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 3.3 SJR 2.762 SNIP 1.316
Web of Science (2014): Impact factor 3.736
Web of Science (2014): Indexed yes
Scopus rating (2013): CiteScore 3.55 SJR 2.813 SNIP 1.326
Web of Science (2013): Impact factor 3.664
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.57 SJR 3.173 SNIP 1.378
Web of Science (2012): Impact factor 3.767
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 3.61 SJR 3.326 SNIP 1.423
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Impact factor 3.774
Mid-IR optical properties of silicon doped InP

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

General information
State: Published
Organisations: Plasmonics and Metamaterials, Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Department of Photonics Engineering, Nanophotonic Devices, St. Petersburg Academic University
Contributors: Panah, M. E. A., Han, L., Norman, K., Pryds, N., Nadtochiy, A., Zhukov, A. E., Lavrinenko, A., Semenova, E.
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Journal: Optical Materials Express
Volume: 7
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, DTU Danchip, Department of Energy Conversion and Storage, Electrofunctional materials, Applied Electrochemistry, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Micro- and Nanotechnology, University of New South Wales
Contributors: Cazzaniga, A. C., Canulescu, S., Ettlinger, R. B., Pryds, N., Hansen, O., Schou, J., Crovetto, A., Hansen, O., Yan, C., Sun, K., Hao, X.
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Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency

General information
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Organisations: Department of Photonics Engineering, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, DTU Danchip, Photovoltaic Materials and Systems, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Micro- and Nanotechnology, University of New South Wales
Releasing cation diffusion in self-limited nanocrystalline defective ceria thin films

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

General information
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Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Electrofunctional materials, Chinese Academy of Sciences
Contributors: Esposito, V., Ni, D. W., Gualandris, F., Pryds, N.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736
Web of Science (2017): Impact factor 2.936
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Web of Science (2016): Impact factor 3.108
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834
Web of Science (2015): Impact factor 3.289
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.87 SJR 1.113 SNIP 0.962
Web of Science (2014): Impact factor 3.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.74 SJR 1.119 SNIP 0.904
Web of Science (2013): Impact factor 3.708
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 2.4 SJR 0.872 SNIP 0.619
Web of Science (2012): Impact factor 2.562
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scavenging of oxygen vacancies at modulation-doped oxide Interfaces: Evidence from oxygen isotope tracing
The introduction of manganite buffer layers, La_{7/8}Sr_{1/8}MnO_3 (LSMO) in particular, at the metallic interface between SrTiO_3 (STO) and another band insulator suppresses the carrier density of the interfacial two-dimensional electron gas (2DEG) and improves significantly the electron mobility. However, the mechanisms underlying the extreme mobility enhancement remain elusive. Herein, we used 18O isotope exchanged SrTiO_3 as substrates to create 2DEG at room temperature with and without the LSMO buffer layer. By mapping the oxygen profile across the interface between STO18 and disordered LaAlO_3 or yttria-stabilized zirconia (YSZ), we provide unambiguous evidence that redox reactions occur at oxide interfaces even grown at room temperature. Moreover, the manganite buffer layer not only suppresses the carrier density but also strongly suppresses the oxygen exchange dynamics of the STO substrate, which likely prevents the reduction of STO during the formation of the 2DEG. The underlying mechanism on the enhanced electron mobility at buffered oxide interfaces is also discussed.

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Suppressed carrier density for the patterned high mobility two-dimensional electron gas at γ-Al_2O_3/SrTiO_3 heterointerfaces
The two-dimensional electron gas (2DEG) at the non-isostructural interface between spinel γ-Al2O3 and perovskite SrTiO3 is featured by a record electron mobility among complex oxide interfaces in addition to a high carrier density up to the order of $10^{15}$ cm$^{-2}$. Herein, we report on the patterning of 2DEG at the γ-Al2O3/SrTiO3 interface grown at 650 °C by pulsed laser deposition using a hard mask of LaMnO3. The patterned 2DEG exhibits a critical thickness of 2 unit cells γ-Al2O3 for the occurrence of interface conductivity, similar to the unpatterned sample. However, its maximum carrier density is found to be approximately $3 \times 10^{13}$ cm$^{-2}$, much lower than that of the unpatterned sample ($\sim 10^{15}$ cm$^{-2}$). Remarkably, a high electron mobility of approximately 3,600 cm$^2$V$^{-1}$s$^{-1}$ was obtained at low temperatures for the patterned 2DEG at a carrier density of $\sim 7 \times 10^{12}$ cm$^{-2}$, which exhibits clear Shubnikov-de Hass quantum oscillations. The patterned high-mobility 2DEG at the γ-Al2O3/SrTiO3 interface paves the way for the design and application of spinel/perovskite interfaces for high-mobility all-oxide electronic devices.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, Nanjing University
Thermodynamic Ground States of Complex Oxide Heterointerfaces

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

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Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
Web of Science (2017): Impact factor 8.097
Transport and excitations in a negative-U quantum dot at the LaAlO$_3$/SrTiO$_3$ interface

In a solid-state host, attractive electron–electron interactions can lead to the formation of local electron pairs which play an important role in the understanding of prominent phenomena such as high $T_c$ superconductivity and the pseudogap phase. Recently, evidence of a paired ground state without superconductivity was demonstrated at the level of single electrons in quantum dots at the interface of LaAlO$_3$ and SrTiO$_3$. Here, we present a detailed study of the excitation spectrum and transport processes of a gate-defined LaAlO$_3$/SrTiO$_3$ quantum dot exhibiting pairing at low temperatures. For weak tunneling, the spectrum agrees with calculations based on the Anderson model with a negative effective charging energy $U$, and exhibits an energy gap corresponding to the Zeeman energy of the magnetic pair-breaking field. In contrast, for strong coupling, low-bias conductance is enhanced with a characteristic dependence on temperature, magnetic field and chemical potential consistent with the charge Kondo effect.

General information

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Number of pages: 7
Tuning the ground state of polar LaAlO$_3$/SrTiO$_3$ interface by an electron sink

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

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, University of Copenhagen
Contributors: Gan, Y., von Soosten, M., Zhang, Y., Niu, W., Christensen, D. V., Sand Jespersen, T., Pryds, N., Chen, Y.
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Tuning the two-dimensional electron liquid at oxide interfaces by buffer-layer-engineered redox reactions
Polar discontinuities and redox reactions provide alternative paths to create two-dimensional electron liquids (2DELs) at oxide interfaces. Herein, we report high mobility 2DELs at interfaces involving SrTiO$_3$ (STO) achieved using polar La$_{7/8}$Sr$_{1/8}$MnO$_3$ (LSMO) buffer layers to manipulate both polarities and redox reactions from disordered overlayers grown at room temperature. Using resonant x-ray reflectometry experiments, we quantify redox reactions from oxide overlayers on STO as well as polarity induced electronic reconstruction at epitaxial LSMO/STO interfaces. The analysis reveals how these effects can be combined in a STO/LSMO/disordered film trilayer system to yield high mobility modulation doped 2DELs, where the buffer layer undergoes a partial transformation from perovskite to brownmillerite structure. This uncovered interplay between polar discontinuities and redox reactions via buffer layers provides a new approach for the design of functional oxide interfaces.

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of British Columbia, Canadian Light Source
Contributors: Chen, Y., Green, R. J., Sutarto, R., He, F., Linderoth, S., Sawatzky, G. A., Pryds, N.
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Web of Science (2017): Indexed yes
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BFI (2015): BFI-level 2
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BFI (2014): BFI-level 2
Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Contributors: Chen, Y., Gan, Y., Christensen, D. V., von Soosten, M., Zhang, Y., Niu, W., Pryds, N.
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Ultra-thin Cu2ZnSnS4 solar cell by pulsed laser deposition

We report on the fabrication of a 5.2% efficiency Cu2ZnSnS4 (CZTS) solar cell made by pulsed laser deposition (PLD) featuring an ultra-thin absorber layer (less than 450 nm). Solutions to the issues of reproducibility and micro-particulate ejection often encountered with PLD are proposed. At the optimal laser fluence, amorphous CZTS precursors with optimal stoichiometry for solar cells are deposited from a single target. Such precursors do not result in detectable segregation of secondary phases after the subsequent annealing step. In the analysis of the solar cell device, we focus on the effects of the finite thickness of the absorber layer. Depletion region width, carrier diffusion length, and optical losses due to incomplete light absorption and back contact reflection are quantified. We conclude that material- and junction quality is comparable to that of thicker state-of-the-art CZTS devices, even though the efficiency is lower due to optical losses.
Universality of electron mobility in LaAlO$_3$/SrTiO$_3$ and bulk SrTiO$_3$

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

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Minnesota, Massachusetts Institute of Technology
Contributors: Trier, F., Reich, K. V., Christensen, D. V., Zhang, Y., Tuller, H. L., Chen, Y., Shklovskii, B. I., Pryds, N.
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When two become one: an insight into 2D conductive oxide interfaces

Recent progress has led to conductance confinement at the interface of complex oxide heterostructures, thereby providing new opportunities to explore nano-electronic as well as nano-ionic devices. In this paper we describe how interfacial contiguity between materials can trigger redox reactions inducing metallic conductivity along the interface of SrTiO$_3$-based heterostructures and create new types of 2 Dimension Electron Gases (2DEG) at the hetero-interface with electron mobility enhancements of more than one order of magnitude higher than those of hitherto investigated perovskite-type interfaces. Furthermore, our recent results, examining strain effects at interfaces, demonstrate the potential of achieving hetero-epitaxial thin films with superior ionic or electronic properties. We also present a novel concept that uncovers a wide variety of possible technological opportunities for materials design utilizing ionic conducting multi-layered heterostructures. These findings hold the potential to pave the way for novel and/or superior all-oxide electronic and ionic devices.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science
A high mobility two-dimensional electron gas at the CaZrO₃/SrTiO₃ heterointerface

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Chen, Y., Trier, F., Christensen, D. V., Linderoth, S., Pryds, N.
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Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2016
**A regenerative elastocaloric heat pump**

A large fraction of global energy use is for refrigeration and air-conditioning, which could be decarbonized if efficient renewable energy technologies could be found. Vapour-compression technology remains the most widely used system to move heat up the temperature scale after more than 100 years; however, caloric-based technologies (those using the magnetocaloric, electrocaloric, barocaloric or elastocaloric effect) have recently shown a significant potential as alternatives to replace this technology due to high efficiency and the use of green solid-state refrigerants. Here, we report a regenerative elastocaloric heat pump that exhibits a temperature span of 15.3K on the water side with a corresponding specific heating power up to 800 W kg\(^{-1}\) and maximum COP (coefficient-of-performance) values of up to 7. The efficiency and specific heating power of this device exceeds those of other devices based on caloric effects. These results open up the possibility of using the elastocaloric effect in various cooling and heat-pumping applications.

**General information**

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana
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- Web of Science (2017): Impact factor 46.859
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- BFI (2016): BFI-level 1
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Research output: Research - peer-review; Journal article – Annual report year: 2016

**A thermoelectric power generating heat exchanger: Part I – Experimental realization**

An experimental realization of a heat exchanger with commercial thermoelectric generators (TEGs) is presented. The power producing capabilities as a function of flow rate and temperature span are characterized for two different commercial heat transfer fluids and for three different thermal interface materials. The device is shown to produce 2W per TEG or 0.22W cm\(^{-2}\) at a fluid temperature difference of 175 °C and a flow rate per fluid channel of 5 L min\(^{-1}\). One experimentally realized design produced 200W in total from 100 TEGs. For the design considered here, the power production is shown to depend more critically on the fluid temperature span than on the fluid flow rate. Finally, the temperature span across the TEG is shown to be 55–75% of the temperature span between the hot and cold fluids. © 2016 Elsevier Ltd. All rights reserved.

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A thermoelectric power generating heat exchanger: Part II – Numerical modeling and optimization

In Part I of this study, the performance of an experimental integrated thermoelectric generator (TEG)-heat exchanger was presented. In the current study, Part II, the obtained experimental results are compared with those predicted by a finite element (FE) model. In the simulation of the integrated TEG-heat exchanger, the thermal contact resistance between the TEG and the heat exchanger is modeled assuming either an ideal thermal contact or using a combined Cooper–Mikic–Yovanovich (CMY) and parallel plate gap formulation, which takes into account the contact pressure, roughness and hardness of the interface surfaces as well as the air gap thermal resistance at the interface. The combined CMY and parallel plate gap model is then further developed to simulate the thermal contact resistance for the case of an interface material. The numerical results show good agreement with the experimental data with an average deviation of 17% for the case without interface material and 12% in the case of including additional material at the interfaces. The model is then employed to evaluate the power production of the integrated system using different interface materials, including graphite, aluminum (Al), tin (Sn) and lead (Pb) in a form of thin foils. The numerical results show that lead foil at the interface has the best performance, with an improvement in power production of 34% compared to graphite foil. Finally, the model predicts that for a certain flow rate, increasing the parallel TEG channels for the integrated systems with 4, 8, and 12TEGs enhances the net power per TEG with average values of 2.5%, 3% and 5%, respectively.© 2016 Elsevier Ltd. All rights reserved.
Challenges in going from 2nd order to 1st order materials in magnetic refrigeration devices

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Bahl, C., Engelbrecht, K., Eriksen, D., Nielsen, K. K., Lei, T., Smith, A., Pryds, N.
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Effects of spark plasma sintering conditions on the anisotropic thermoelectric properties of bismuth antimony telluride

Bismuth antimony telluride (Bi$_{x}$Sb$_{2-x}$Te$_{3}$, 0.4 < x < 0.6) is one of the best and most-used p-type semiconductor materials for near-room-temperature thermoelectric power generation. In this work, p-type Bi$_{0.4}$Sb$_{1.6}$Te$_{3}$ samples were prepared under various conditions (temperature, holding time, and ramp-rate) using spark plasma sintering (SPS). The effects of SPS conditions on the anisotropic thermoelectric properties and microstructure evolutions were systematically investigated. The change of sintering temperature showed stronger influence than other sintering parameters to the resulting thermoelectric properties. Samples sintered over the temperature range between 653 K and 773 K showed significant differences in the degrees of orientations. The change was mainly caused by grain growth and re-orientation. Despite of the anisotropy, zT value as high as 1.2 to 1.3 was achieved over the temperature range of 300 to 360 K by directly using commercial power sintered at 723 and 773 K. The sintering profiles and microstructure evolutions during SPS were illustrated and the thermoelectric properties as a function of the degrees of orientations were shown and discussed in detail.

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization, Technical University of Denmark, Fraunhofer Institute for Material and Beam Technology
Contributors: Han, L., Hegelund Spangsdorf, S., Van Nong, N., Le, T. H., Zhang, Y., Pham, H. N., Chen, Y., Roch, A., Stepien, L., Pryds, N.
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Web of Science (2016): Impact factor 3.108
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834
Web of Science (2015): Impact factor 3.289
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.87 SJR 1.113 SNIP 0.962
Web of Science (2014): Impact factor 3.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.74 SJR 1.119 SNIP 0.904
Web of Science (2013): Impact factor 3.708
Effects of surface finish and mechanical training on Ni-Ti sheets for elastocaloric cooling

Elastocaloric cooling has emerged as a promising alternative to vapor compression in recent years. Although the technology has the potential to be more efficient than current technologies, there are many technical challenges that must be overcome to realize devices with high performance and acceptable durability. We study the effects of surface finish and training techniques on dog bone shaped polycrystalline samples of NiTi. The fatigue life of several samples with four different surface finishes was measured and it was shown that a smooth surface, especially at the edges, greatly improved fatigue life. The effects of training both on the structure of the materials and the thermal response to an applied strain was studied. The load profile for the first few cycles was shown to change the thermal response to strain, the structure of the material at failure while the final structure of the material was weakly influenced by the surface finish.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization
Contributors: Engelbrecht, K., Tusek, J., Sanna, S., Eriksen, D., Mishin, O., Bahl, C., Pryds, N.
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Scopus rating (2016): CiteScore 3.67 SJR 2.177 SNIP 1.151
Web of Science (2016): Impact factor 4.335
Web of Science (2016): Indexed yes
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Bibliographical note
Elastocaloric effect of a Ni-Ti plate to be applied in a regenerator-based cooling device

The aim of this article is to analyze the elastocaloric effect of a commercial Ni-Ti plate for its application in a cooling device. In the first part, the article shows numerical results of the cooling characteristics of a regenerator-based elastocaloric cooling device with different thickness of the Ni-Ti plates based on a previously developed numerical model. It is shown that such a device (with a plate thickness of 0.1 mm) can produce a specific cooling power up to 7 kW/kg and coefficient of performance values up to 5 at the 30 K of the temperature span. In the second part of the article, a testing and analysis of the elastocaloric effect of the Ni-Ti plate using infrared thermography is shown. Prior to the elastocaloric testing, the sample was mechanically polished and subjected to 200 loading–unloading cycles at a slow strain-rate and 10,000 loading–unloading cycles at high strain-rate to stabilize its superelastic behavior and evaluate its fatigue life. When the functional and structural stability was reached and relatively good fatigue resistance was proven, the elastocaloric effect of the sample was studied with an infrared camera as a function of strain-rate and applied strain. It is shown that the adiabatic conditions are well approximated at strain-rates above 0.1 s⁻¹. The largest adiabatic temperature change of 14 K during loading and 12.5 K during unloading were measured at the applied strain of 4.2% (at a strain-rate of 0.33 s⁻¹). The homogeneity of the elastocaloric effect and the temperature irreversibilities during unloading are presented and discussed. It can be concluded that thin Ni-Ti plates with suitable austenitic finish temperature are good candidates to be applied in a proof-of-concept regenerator-based cooling device.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.01
Web of Science (2016): Impact factor 0.88
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Web of Science (2015): Impact factor
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.514 SNIP 0.731
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BFI (2013): BFI-level 1
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Web of Science (2012): Indexed yes
Electric field control of the $\gamma$-Al$_2$O$_3$/SrTiO$_3$ interface conductivity at room temperature

Controlling interfaces using electric fields is at the heart of modern electronics. The discovery of the conducting interface between the two insulating oxides LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) has led to a number of interesting electric field-dependent phenomena. Recently, it was shown that replacing LAO with a spinel $\gamma$-Al$_2$O$_3$ (GAO) allows a good pseudo-epitaxial film growth and high electron mobility at low temperatures. Here, we show that the GAO/STO interface resistance, similar to LAO/STO, can be tuned by orders of magnitude at room temperature using the electric field of a backgate. The resistance change is non-volatile, bipolar, and can be tuned continuously rather than being a simple on/off switch. Exposure to light significantly changes the capabilities to tune the interface resistance. High- and low-resistive states are obtained by annihilation and creation, respectively, of free $n$-type carriers, and we speculate that electromigration of oxygen vacancies is the origin of the tunability.

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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Impact factor 3.411
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.47 SJR 1.499 SNIP 1.226
Web of Science (2015): Impact factor 3.142
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.25 SJR 1.861 SNIP 1.492
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.77 SJR 2.146 SNIP 1.633
Web of Science (2013): Impact factor 3.515
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.76 SJR 2.57 SNIP 1.739
Web of Science (2012): Impact factor 3.794
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.04 SJR 2.814 SNIP 1.917
Web of Science (2011): Impact factor 3.844
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Impact factor 3.841
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.012 SNIP 1.916
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.755 SNIP 2.353
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.992 SNIP 2.367
Web of Science (2004): Indexed yes
Evidence for lattice-polarization-enhanced field effects at the SrTiO$_3$-based heterointerface

Electrostatic gating provides a powerful approach to tune the conductivity of the two-dimensionalelectron liquid between two insulating oxides. For the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface, such gating effect could be further enhanced by a strong lattice polarization of STO caused by simultaneous application of gate field and illumination light. Herein, by monitoring the discharging process upon removing the gate field, we give firm evidence for the occurrence of this lattice polarization at the amorphous-LaAlO$_3$/SrTiO$_3$ interface. Moreover, we find that the lattice polarization is accompanied with a large expansion of the out-of-plane lattice of STO. Photo excitation affects the polarization process by accelerating the field-induced lattice expansion. The present work demonstrates the great potential of combined stimuli in exploring emergent phenomenon at complex oxide interfaces.
Evidence of weak superconductivity at the room-temperature grown LaAlO$_3$/SrTiO$_3$ interface

The two-dimensional electron gas at the crystalline LaAlO$_3$/SrTiO$_3$ (c-LAO/STO) interface has sparked large interest due to its exotic properties, including an intriguing gate-tunable superconducting phase. While there is growing evidence of pronounced spatial inhomogeneity in the conductivity at STO-based interfaces, the consequences for superconductivity remain largely unknown. We study interfaces based on amorphous LAO top layers grown at room temperature (a-LAO/STO) and demonstrate a superconducting phase similar to c-LAO/STO, however, with a gate-tunable critical temperature of 460 mK. The dependence of the superconducting critical current on temperature, magnetic field, and back-gate-controlled doping is found to be consistently described by a model of a random array of Josephson-coupled superconducting domains.
Experimental performance evaluation of sintered Gd spheres packed beds

Research in magnetic refrigeration heavily relies on the use of packed spheres in regenerators, however little investigation to verify that such non-monolithic arrangements guarantee a sufficiently constrained structure has yet been performed. This work presents a preliminary comparison of the performance of AMRs consisting of Gd spheres with diameters ranging from 450-550 microns partially sintered by Spark Plasma Sintering (SPS) to similar spheres, sorted in the same
size range and from the same batch, but merely packed. Pressure drop is compared at uniform temperature and at a range of heat rejection temperatures and temperature spans. Performance is compared in terms of temperature span at a range of heat rejection temperatures (295-308 K) and 0 and 10 W cooling loads. Results show a moderate increase of pressure drop with the sintered spheres, while temperature spans were consistently 2.5-5 K smaller. These results are coherent with previously presented results [1].

General information
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Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials, University of Victoria BC
Contributors: Tura, A., Nielsen, K. K., Van Nong, N., Pryds, N., Trevizoli, P. V., Christiaanse, T. V., Teyber, R., Rowe, A.
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Source-ID: 2358372821
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Formation of copper tin sulfide films by pulsed laser deposition at 248 and 355 nm
The influence of the laser wavelength on the deposition of copper tin sulfide (CTS) and SnS-rich CTS with a 248-nm KrF excimer laser (pulse length τ = 20 ns) and a 355-nm frequency-tripled Nd:YAG laser (τ = 6 ns) was investigated. A comparative study of the two UV wavelengths shows that the CTS film growth rate per pulse was three to four times lower with the 248-nm laser than the 355-nm laser. SnS-rich CTS is more efficiently ablated than pure CTS. Films deposited at high fluence have submicron and micrometer size droplets, and the size and area density of the droplets do not vary significantly from 248 to 355 nm deposition. Irradiation at low fluence resulted in a non-stoichiometric material transfer with significant Cu deficiency in the as-deposited films. We discuss the transition from a non-stoichiometric material transfer at low fluence to a nearly stoichiometric ablation at high fluence based on a transition from a dominant evaporation regime to an ablation regime.

General information
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Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Contributors: Ettlinger, R. B., Crovetto, A., Canulescu, S., Cazzaniga, A. C., Ravnkilde, L., Youngman, T. H., Hansen, O., Pryds, N., Schou, J.
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BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.62 SJR 0.481 SNIP 0.699
Web of Science (2017): Impact factor 1.604
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
High ionic conductivity in confined bismuth oxide-based heterostructures

Bismuth trioxide in the cubic fluorite phase (δ-Bi2O3) exhibits the highest oxygen ionic conductivity. In this study, we were able to stabilize the pure δ-Bi2O3 at low temperature with no addition of stabilizer but only by engineering the interface, using highly coherent heterostructures made of alternative layers of δ-Bi2O3 and Yttria Stabilized Zirconia (YSZ), deposited by pulsed laser deposition. The resulting [δ-Bi2O3=YSZ] heterostructures are found to be stable over a wide temperature range (500-750 °C) and exhibits stable high ionic conductivity over a long time comparable to the value of the pure δ-Bi2O3, which is approximately two orders of magnitude higher than the conductivity of YSZ bulk.

Infrared ellipsometry study of the confined electrons in a high-mobility γ-Al2O3/SrTiO3 heterostructure

With infrared ellipsometry we studied the response of the confined electrons in γ-Al2O3/SrTiO3 (GAO/STO) heterostructures in which they originate predominantly from oxygen vacancies. From the analysis of a so-called Berreman mode, that develops near the highest longitudinal optical phonon mode of SrTiO3, we derive the sheet carrier density, Ns, the mobility, μ, and the depth profile of the carrier concentration. Notably, we find that Ns and the shape of the depth profile are similar as in LaAlO3/SrTiO3 (LAO/STO) heterostructures for which the itinerant carriers are believed to arise from a polar discontinuity. Despite an order of magnitude higher mobility in GAO/STO, as obtained from transport measurements, the derived mobility in the infrared range exhibits only a twofold increase. We interpret this finding in terms...
of the polaronic nature of the confined charge carriers in GAO/STO and LAO/STO which leads to a strong, frequency-dependent interaction with the STO phonons.
Material transfer in Pulsed Laser Deposition of the solar cell materials Cu$_2$SnS$_3$ and Cu$_2$ZnSnS$_4$.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, DTU Danchip, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Micro- and Nanotechnology
Contributors: Cazzaniga, A. C., Canulescu, S., Crovetto, A., Ettlinger, R. B., Pryds, N., Hansen, O., Schou, J.
Number of pages: 1
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Event: Abstract from Annual Meeting of the Danish Physical Society, Middelfart, Denmark.
Electronic versions: abstract_DFS_2016_Andcan.pdf
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2017

New Insights into the Creation of High-Mobility Two-Dimensional Electron Gas at Oxide Interfaces: Control of Interfacial Redox Reactions by an Electron Sink

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of British Columbia, Canadian Light Source, Chinese Academy of Sciences
Contributors: Chen, Y., Green, R., Trier, F., Christensen, D. V., Sutarto, R., He, F., von Soosten, M., Zhang, Y., Linderoth, S., Pryds, N.
Number of pages: 1
Publication date: 2016
Peer-reviewed: Yes
Event: Abstract from 23rd International Workshop on Oxide Electronics, Nanjing, China.
Electronic versions:
On the Challenges of Reducing Contact Resistances in Thermoelectric Generators Based on Half-Heusler Alloys

A method using fast hot pressing to join half-Heusler (HH) thermoelectric materials directly to an electrical current collector (Ag electrode) without using a third filler material is introduced. The compositions of the HH alloys used are Hf0.5Zr0.5CoSn0.2Sb0.8 and Ti0.6Hf0.4NiSn for p- and n-type, respectively. Using this method, the quality of the HH–electrode contacts is improved due to their low electrical contact resistance and less reaction–diffusion layer. The microstructure and chemical composition of the joints were examined using a scanning electron microscope equipped with energy-dispersive x-ray analysis. The electrical characteristics of the interfaces at the contacts were studied based on electrical contact resistance and Seebeck scanning microprobe measurements. In this paper, we show that joining the HH to a Ag electrode directly using fast hot pressing resulted in lower contact resistance and better performance compared with the method of using active brazing filler alloy.
Pulsed Laser Deposition (PLD) of the Solar Cell Materials CZTS and CTS

**General information**

*State:* Published

*Organisations:* Department of Photonics Engineering, Photovoltaic Materials and Systems, DTU Danchip, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Micro- and Nanotechnology, Department of Energy Conversion and Storage, Electrofunctional materials

*Contributors:* Schou, J., Cazzaniga, A. C., Canulescu, S., Ettlinger, R. B., Crovetto, A., Engberg, S. L. J., Hansen, O., Pryds, N.

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*Publication date:* 2016

*Peer-reviewed:* Yes

*Event:* Abstract from 2016 MRS Spring Meeting & Exhibit, Phoenix, United States.

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Abstract_MRS_2016.pdf

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**Quantization of Hall Resistance at the Metallic Interface between an Oxide Insulator and SrTiO3**

The two-dimensional metal forming at the interface between an oxide insulator and SrTiO3 provides new opportunities for oxide electronics. However, the quantum Hall effect, one of the most fascinating effects of electrons confined in two dimensions, remains underexplored at these complex oxide heterointerfaces. Here, we report the experimental observation of quantized Hall resistance in a SrTiO3 heterointerface based on the modulation-doped amorphous-LaAlO3/SrTiO3 heterostructure, which exhibits both high electron mobility exceeding 10,000 cm²/V s and low carrier density on the order of ~10¹² cm⁻². Along with unambiguous Shubnikov-de Haas oscillations, the spacing of the quantized Hall resistance suggests that the interface is comprised of a single quantum well with ten parallel conducting two-dimensional subbands. This provides new insight into the electronic structure of conducting oxide interfaces and represents an important step towards designing and understanding advanced oxide devices.
Quantum and field effects of oxide heterostructures

The interface between two materials can show radically different properties than either of the bulk parent materials. This is not the least true for oxide interfaces, which can display multiple physical functionalities thus making them ideal for the realisation of so-called multi-plexed devices. In these multi-plexed devices, several inputs are translated into several outputs through the multiple physical functionalities. A highly prominent example of such an oxide interface is the one between LaAlO₃ and SrTiO₃. Although both LaAlO₃ and SrTiO₃ in the bulk are electrically insulating and non-magnetic, their interface nonetheless shows attractive properties such as metallic conductivity, superconductivity and ferromagnetism. This thesis will provide an extensive review of the literature concerning the interface metal present in LaAlO₃/SrTiO₃ as well as in other SrTiO₃-based heterostructures. Through this review, several open questions will be revealed, which constitute the scientific aims of this thesis. These open questions will subsequently be addressed through the work presented in the articles that were published during the course of this Ph.D. study. In the review of these published articles, the important aspects of sample preparation will initially be covered. Here, the growth of amorphous-LaAlO₃ on SrTiO₃ will be addressed in a modified pulsed laser deposition setup. This is followed by an investigation of two high-electron mobility interfaces in SrTiO₃-based heterostructures. Specifically, these interfaces are the ones between CaZrO₃/SrTiO₃ and amorphous-LaAlO₃/(La, Sr)MnO₃/SrTiO₃. The sample preparation section is ended by outlining a patterning strategy for the high-electron mobility interface at amorphous-LaAlO₃/(La, Sr)MnO₃/SrTiO₃. Subsequently, the effects of electrostatic gating is studied in two different SrTiO₃-based heterostructures. Here, it is shown that the interface between amorphous-LaAlO₃ and SrTiO₃ is superconducting with a larger critical transition temperature than that in LaAlO₃/SrTiO₃. For γ-Al₂O₃/SrTiO₃, it is shown that non-volatile bipolar resistance switching is possible with a gradual tuning of the interface conductivity. Finally, the so-called quantum Hall effect is demonstrated at the interface between amorphous-LaAlO₃/(La, Sr)MnO₃/SrTiO₃. The manifestation of the quantum Hall effect reveals that the interface conductivity is comprised of several subbands conducting in parallel. An outlook will be provided at the end of the thesis judging the research as well as development of oxide electronics and multi-plexed devices.

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Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Copenhagen
Contributors: Trier, F., Pryds, N., Chen, Y., Sand Jespersen, T.
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Scandium-doped zinc cadmium oxide as a new stable n-type oxide thermoelectric material

Scandium-doped zinc cadmium oxide (Sc-doped ZnCdO) is proposed as a new n-type oxide thermoelectric material. The material is sintered in air to maintain the oxygen stoichiometry and avoid instability issues. The successful alloying of CdO with ZnO at a molar ratio of 1:9 significantly reduced the thermal conductivity by up to 7-fold at room temperature. By carefully selecting the Sc-dopant concentrations, a high power factor of $7.1 \times 10^{-4}$ W m$^{-1}$ K$^{-2}$ at 1173 K could be obtained. Therefore, the highest ZT of 0.3 at 1173 K was achieved for the Zn$_{0.9}$Cd$_{0.1}$Sc$_{0.01}$O$_{1.015}$ sample, and it has so far one of the highest ZT values among those reported for ZnO based thermoelectric materials over the temperature range, e.g., its ZT value at 300 K, which is 0.012, is over 1 order of magnitude higher than that of the state-of-the-art nanostuctured Al-doped ZnO, which is 0.0013. It suggests that this material is a good candidate for improving the overall conversion efficiencies in oxide thermoelectric modules. Meanwhile, Sc-doped ZnCdO is robust in air at high temperatures, whereas other n-type materials, such as Al-doped ZnO, will experience rapid degradation of their electrical conductivity and ZT.
Silicon doped InP as an alternative plasmonic material for mid-infrared

Silicon-doped InP is grown on top of semiinsulating iron-doped and sulfur-doped InP substrates by metalorganic vapor phase epitaxy (MOVPE), and the growth parameters are adjusted to obtain various free carrier concentrations from $1.05 \times 10^{19}$ cm$^{-3}$ up to $3.28 \times 10^{19}$ cm$^{-3}$. Midinfrared (IR) reflection spectra of the samples with different carrier concentrations are used to retrieve pertaining dielectric functions as the key factor for understanding plasmonic behavior of InP:Si in the mid-IR wavelength range.

The 2016 oxide electronic materials and oxide interfaces roadmap

Oxide electronic materials provide a plethora of possible applications and offer ample opportunity for scientists to probe into some of the exciting and intriguing phenomena exhibited by oxide systems and oxide interfaces. In addition to the already diverse spectrum of properties, the nanoscale form of oxides provides a new dimension of hitherto unknown phenomena due to the increased surface-volume ratio. Oxide electronic materials are becoming increasingly important in a wide range of applications including transparent electronics, optoelectronics, magnetoelectronics, photonics, spintronics, thermoelectrics, piezoelectrics, power harvesting, hydrogen storage and environmental waste management. Synthesis and fabrication of these materials, as well as processing into particular device structures to suit a specific application is still a challenge. Further, characterization of these materials to understand the tunability of their properties and the novel properties that evolve due to their nanostructured nature is another facet of the challenge. The research related to the oxide electronic field is at an impressionable stage, and this has motivated us to contribute with a roadmap on ‘oxide electronic materials and oxide interfaces’. This roadmap envisages the potential applications of oxide materials in cutting edge technologies and focuses on the necessary advances required to implement these materials, including both conventional and novel techniques for the synthesis, characterization, processing and fabrication of nanostructured oxides and oxide-based devices. The contents of this roadmap will highlight the functional and correlated properties of oxides in bulk, nano, thin film, multilayer and heterostructure forms, as well as the theoretical considerations behind both present and future applications in many technologically important areas as pointed out by Venkatesan. The contributions in this roadmap span several thematic groups which are represented by the following authors: novel field effect transistors and bipolar devices by Fortunato, Grundmann, Boschker, Rao, and Rogers; energy conversion and saving by Zaban, Weidenkaff, and Murakami; new opportunities of photonics by Fompheyrine, and Zuniga-Perez; multiferroic materials including novel phenomena by Ramesh, Spaldin, Mertig, Lorenz, Srinivasan, and Pellar; and concepts for topological oxide electronics by Kawasaki, Pentcheva, and Gegenwart. Finally, Miletto Granozio presents the European action ‘towards oxide-based electronics’ which develops an oxide electronics roadmap with emphasis on future nonvolatile memories and the required technologies. In summary, we do hope that this oxide roadmap appears as an interesting up-to-date snapshot on one of the most exciting and active areas of solid state physics, materials science, and chemistry, which even after many years of very successful development shows in short intervals novel insights and achievements. Guest editors: M S Ramachandra Rao and Michael Lorenz.
Understanding the Thermodynamic Properties of the Elastocaloric Effect Through Experimentation and Modelling

This paper presents direct and indirect methods for studying the elastocaloric effect (eCE) in shape memory materials and its comparison. The eCE can be characterized by the adiabatic temperature change or the isothermal entropy change (both as a function of applied stress/strain). To get these quantities, the evaluation of the eCE can be done using either direct methods, where one measures (adiabatic) temperature changes or indirect methods where one can measure the stress–strain–temperature characteristics of the materials and from these deduce the adiabatic temperature and isothermal entropy changes. The former can be done using the basic thermodynamic relations, i.e. Maxwell relation and Clausius–Clapeyron equation. This paper further presents basic thermodynamic properties of shape memory materials, such as the adiabatic temperature change, isothermal entropy change and total entropy–temperature diagrams (all as a function of temperature and applied stress/strain) of two groups of materials (Ni–Ti and Cu–Zn–Al alloys) obtained using indirect methods through phenomenological modelling and Maxwell relation. In the last part of the paper, the basic definition of the efficiency of the elastocaloric thermodynamic cycle (coefficient of performance) is defined and discussed.

General information
- State: Published
- Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana, University of Barcelona
- Contributors: Tušek, J., Engelbrecht, K., Mañosa, L., Vives, E., Pryds, N.
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- Peer-reviewed: Yes

Publication information
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- Volume: 2
- Issue number: 4
- ISSN (Print): 2199-384X
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- DOIs:
A study of thermoelectric $\beta$-Zn$_4$Sb$_3$ under thermal cycling and large temperature gradients

Band bending and alignment at the spinel/perovskite $\gamma$-Al$_2$O$_3$/SrTiO$_3$ heterointerface

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, TEGnology ApS, Aarhus University
Contributors: Le, T. H., Van Nong, N., Han, L., Brummerstedt Iversen, B., Yin, H., Pryds, N.
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Article number: PA188
Electronic versions:
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Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Universität Würzburg, Helmholtz–Zentrum Berlin für Materialien und Energie
Contributors: Schütz, P., Pfaff, F., Scheiderer, P., Chen, Y., Pryds, N., Gorgoi, M., Sing, M., Claessen, R.
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ISSN (Print): 0163-1829
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Impact factor 3.836
Web of Science (2016): Indexed yes
Scopus rating (2015): CiteScore 2.8 SJR 2.377 SNIP 1.13
Web of Science (2015): Impact factor 3.718
Web of Science (2015): Indexed yes
Chalcogenide compounds made by pulsed laser deposition at 355 and 248 nm

Thin films made by pulsed laser deposition may differ depending on the laser wavelength. We compared ZnS, Cu2SnS3 and a target enriched with SnS relative to Cu2SnS3 using 355 nm and 248 nm lasers

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, DTU Danchip, Department of Energy Conversion and Storage,
Characterization of the contact between Bi2Te3-based materials and lead-free solder alloy under thermal cycling

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Van Nong, N., Le, T. H., Han, L., Pham, H. N., Pryds, N.
Publication date: 2015

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Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
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Electronic versions:
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Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Charge transfer induced modulation doping of two-dimensional electron gas at complex oxide interfaces

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State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Chen, Y., Trier, F., Christensen, D. V., Linderoth, S., Pryds, N.
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Event: Abstract from TO-BE Spring Meeting 2015, Aveiro, Portugal.
Electronic versions:
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Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015

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 SrTiO3-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 CaZrO3/SrTiO3. Remarkably, this heterointerface is atomically sharp and exhibits a high electron mobility exceeding 60 000 cm2 V−1 s−1 at low temperatures. The 2DEG carrier density exhibits a critical dependence on the film thickness, in good agreement with the polarization induced 2DEG scheme.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Center for Electron Nanoscopy, Imaging and Structural Analysis, Atomic Scale Materials Modelling, University of Copenhagen
Pages: 1849–1854
Design and experimental tests of a rotary active magnetic regenerator prototype

A rotary active magnetic regenerator (AMR) prototype with efficiency and compact design as focus points has been designed and built. The main objective is to demonstrate improved efficiency for rotary devices by reducing heat leaks from the environment and parasitic mechanical work losses while optimizing the utilization of the magnetized volume. Heat transfer calculations combined with 1D AMR modeling have revealed the necessity for an insulating air gap between magnet and regenerator when designing for high efficiency. 2D finite difference AMR modeling capturing the interplay between heat transfer fluid flow and an inhomogenous time-varying magnetic field in the individual regenerator beds has been used in the design process. For one operating point a COP of 3.1 at a temperature span of 10.2 K and a cooling power of 103W were measured. Major issues limiting the performance have been identified and improvements are outlined for future work. © 2015 Elsevier Ltd and IIR. All rights reserved.
Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery

Energy safety is a vital issue of the global future. Together with developing renewable and eco-friendly energy sources, recovering waste energy is no less of an important issue. It is estimated that 60% of energy converted in most of today’s energy processes nowadays is waste, mainly in the form of heat. Using thermoelectric generators, which convert heat into electricity, is a promising way to recover waste energy. However, the efficiency of thermal-to-electricity converters needs to be improved in order to be widely applied in practice. Despite the fact that significant amount of efforts have been focused on material development, realizing high efficient thermoelectric generators from such well-developed materials is still limited. Moreover, no single thermoelectric material could withstand the wide temperature range required to boost efficiency of TEGs. By segmentation of different TE materials which operate optimally in each temperature range, this study aims at developing high performance segmented TEGs for medium-high (450 – 850 K) temperature application. The research is focused on the challenges in joining and minimizing the contact resistances between different TE materials and with metal electrode.

One-dimensional numerical modeling was employed to design and predict the efficiency of segmented materials built up from most of today’s state-of-the-art thermoelectric materials. Combinations of materials that would deliver the highest conversion efficiency in different temperature ranges of 300 – 700, and 900 – 1100 K are considered. The obtained results reveals that segmented thermoelectric generator comprising of Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe/SiGe as p-leg and either segmented Bi2Te3/PbTe/SiGe or Bi2Te3/Ba0.08La0.05Yb0.04Co4Sb12/La3Te4 as n-leg working in 300 – 1100 K temperature range could achieve a maximum efficiency of 18.2 %. In lower working temperature ranges of 300 – 700 and 300 – 900 K, the maximum efficiencies are 13.5 and 16.6 %, respectively for segmented TEGs of p-legBi0.6Sb1.4Te3/TAGS ((AgSbTe)0.15(GeTe)0.85) with n-leg Bi2Te3/PbTe and p-leg Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe with n-leg Bi2Te3/PbTe/SiGe. The results could provide a guideline to develop high efficiency segmented thermoelectric generators. Based on these theoretical results, segmentation of half-Heusler alloys and Bi2Te3 materials was selected for further study.

Firstly, the joining between thermoelectric p- and n-type half-Heusler (HH) alloys and silver electrode at hot side was developed. A fast-hot pressing method was introduced to directly join the HH materials with silver interconnecting layer.
The method was also compared with the conventional joining method where a third material is used as filler. Microstructures and interfacial chemical evolution at the joining interfaces were investigated using scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The transport properties of the joint, including thermopower across the interfaces and contact resistance as a function of temperature were studied. With fast hot pressing method, the contact resistance between HH alloys and Ag-electrode could be significantly reduced by about 50%. Moreover, by avoiding a third filler material, the method limits the formation of new phases at contact interface which might degrade the overall thermoelectric properties. This work is a crucial step to make segmented HH/BiTe TEG.

Then, p- and n-type segmented legs of bismuth tellurides and half-Heusler alloys were built and characterized. Segmentation of bismuth tellurides to half-Heusler/Ag was processed at temperature 493 K, pressure 30 MPa in vacuum using Ag10Sn90 solder as filler. Interface microstructural evolution and thermoelectric properties of segmented legs were then investigated. The contact resistance of the join parts as a function of temperature was measured from room temperature to 473 K. Numerical modeling was used to evaluate the influence of measured contact resistances on the final power generating properties of the obtained segmented legs and their unicouple. Under working temperature from 323 to 873 K, the obtained p-segmented legs could deliver a power density of 0.3 Wcm-2 and maximum voltage of 115 mV. With the same condition, the power density and maximum voltage generated by n-segmented leg were 0.25 Wcm-2 and 102 mV. These values are significantly smaller than calculation data. The reason is possibly due to the contact between BiTe and electrode at the cold end, thus improvement of the cold side contact was made. At temperature gradient of 498 K, the maximum power density of the improved n-segmented leg was 0.8 Wcm-2, giving a maximum efficiency of 4.5%.
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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
Web of Science (2015): Impact factor 3.014
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.13 SJR 1.117 SNIP 1.632
Web of Science (2014): Impact factor 2.999
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.73 SJR 1.059 SNIP 1.583
Web of Science (2013): Impact factor 2.726
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.43 SJR 1.246 SNIP 1.57
Web of Science (2012): Impact factor 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.41 SJR 1.164 SNIP 1.463
Web of Science (2011): Impact factor 2.289
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
Web of Science (2010): Impact factor 2.138
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.956 SNIP 1.372
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
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
Scopus rating (2005): SJR 1.088 SNIP 1.208
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.922 SNIP 1.354
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.949 SNIP 1.051
Scopus rating (2002): SJR 0.733 SNIP 1.063
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.634 SNIP 0.966
Scopus rating (2000): SJR 0.707 SNIP 0.938
Scopus rating (1999): SJR 0.744 SNIP 0.927
Elastocaloric cooling device: Materials and modeling
In the last decade we have witnessed the development of alternative solid-state cooling technologies based on so-called ferroic (caloric) effects. A large effort nowadays is devoted to investigating solid-state refrigeration using the magnetocaloric effect (change of temperature upon application of a magnetic field). However, the possibility of inducing a thermodynamic transition by means of mechanical stress (martensitic transformation), i.e. the elastocaloric effect in superelastic materials, opens up new routes for solid-state refrigeration. In the recent years a large elastocaloric effect was demonstrated in Ni-Ti-based, Cu-based as well as Fe-based shape memory alloys. Although these studies showed a great potential of the elastocaloric effect, there has not yet been much activities on development of elastocaloric cooling devices. Some ideas on elastocaloric cooling device have already been presented, but there is still a lack of knowledge and information about its actual cooling potential.

Elastocaloric effect of Ni-Ti wire for application in a cooling device
We report on the elastocaloric effect of a superelastic Ni-Ti wire to be used in a cooling device. Initially, each evaluated wire was subjected to 400 loading/unloading training cycles in order to stabilize its superelastic behavior. The wires were trained at different temperatures, which lead to different stabilized superelastic behaviors. The stabilized (trained) wires were further tested isothermally (at low strain-rate) and adiabatically (at high strain-rate) at different temperatures (from 312 K to 342 K). We studied the impact of the training temperature and resulting superelastic behavior on the adiabatic temperature changes. The largest measured adiabatic temperature change during loading was 25 K with a corresponding 21K change during unloading (at 322 K). A special focus was put on the irreversibilities in the adiabatic temperature changes between loading and unloading. It was shown that there are two sources of the temperature irreversibilities: the hysteresis (and related entropy generation) and the temporary residual strain immediately after unloading, respectively. The latter results in the temporary bending of the wire and reduced negative adiabatic temperature change. The paper also shows the impact of the applied strain on the adiabatic temperature changes as well as the distribution of the elastocaloric effect over the wire during loading in the case of two wires trained at different temperatures and the virgin wire, respectively. In the end, we propose guidelines about the required material properties for an efficient elastocaloric cooling device. © 2015 AIP Publishing LLC.
Enhancement of the chemical stability in confined δ-Bi₂O₃

Bismuth-oxide-based materials are the building blocks for modern ferroelectrics, multifunctionals, gas sensors, light photocatalysts, and fuel cells. Although the cubic fluorite δ-phase of bismuth oxide (δ-Bi₂O₃) exhibits the highest conductivity of known solid-state oxygen ion conductors, its instability prevents use at low temperature. Here we demonstrate the possibility of stabilizing δ-Bi₂O₃ using highly coherent interfaces of alternating layers of Er₂O₃-stabilized δ-Bi₂O₃ and Gd₂O₃-doped CeO₂. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for Bi₂O₃-based materials, is achieved. Even more interestingly, at low oxygen partial pressure the layered material shows anomalous high conductivity, equal or superior to pure δ-Bi₂O₃ in air. This suggests a strategy to design and stabilize new materials that are comprised of intrinsically unstable but high-performing component materials.
Experimental Studies with an Active Magnetic Regenerating Refrigerator

Experimental results for an active magnetic regenerator (AMR) are presented. The focus is on whether or not it pays off to partly substitute soft magnetic material with non-magnetic insulation in a flux-conducting core in the magnet system. Such a substitution reduces losses due to heat conduction and eddy currents, but also reduces the magnetic field. Two different cores were tested in the AMR system with different cooling loads and it is shown, that in the present case, replacing half of the iron with insulation lead to an average reduction in temperature span of 14%, but also a small decrease in COP, hence the substitution did not pay off. Furthermore, it is shown experimentally, that small imbalances in the heat transfer fluid flow greatly influence the system performance. A reduction of these imbalances through valve adjustments resulted in an
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

The discovery of two-dimensional electron gases (2DEGs) at the interface between two insulating complex oxides, such as LaAlO3 (LAO) or gamma-Al2O3 (GAO) epitaxially grown on SrTiO3 (STO), provides an opportunity for developing all-oxide electronic devices. These 2DEGs at complex oxide interfaces involve many-body interactions and give rise to a rich set of phenomena, for example, superconductivity, magnetism, tunable metal-insulator transitions, and phase separation. However, large enhancement of the interfacial electron mobility remains a major and long-standing challenge for fundamental as well as applied research of complex oxides. Here, we inserted a single unit cell insulating layer of polar La1-xSr0.25MnxO3 (x=0, 1/8, and 1/3) at the interface between disordered LaAlO3 and crystalline SrTiO3 created at room temperature. We find that the electron mobility of the interfacial 2DEG is enhanced by more than two orders of magnitude. Our in-situ and resonant x-ray spectroscopic in addition to transmission electron microscopy results indicate that the manganite layer undergoes unambiguous electronic reconstruction and leads to modulation doping of such atomically engineered complex oxide heterointerfaces. At low temperatures, the modulation-doped 2DEG exhibits clear Shubnikov-de Haas oscillations and the initial manifestation of the quantum Hall effect, demonstrating an unprecedented high-mobility and low electron density oxide 2DEG system. These findings open new avenues for oxide electronics.
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen


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Peer-reviewed: Yes
Event: Abstract from 22nd International Workshop on Oxide Electronics, Paris, France.
Electronic versions: Extreme_mobility_enhancement.pdf
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Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

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Research output: Research › Poster – Annual report year: 2015

Functionally Graded Ceramics Fabricated with Side-by-Side Tape Casting for Use in Magnetic Refrigeration

Functionally graded ceramic tapes have been fabricated by a side-by-side tape casting technique. This study shows the possibility and describes the main principles of adjacent coflow of slurries resulting in formation of thin plates of graded ceramic material. Results showed that the small variations of solvent and binder system concentrations have a substantial effect on slurry viscosity. Varying these parameters showed that side-by-side tape casting with a well-defined interface area is possible for slurries with viscosities above 3500 mPa s at a casting shear rate of 3.3 s⁻¹. As it was expected, the choice of de-bindering and sintering regimes significantly influences crack formation, and a three-step heating programme was found to result in tapes of the highest quality. The interface regions of green graded tapes were investigated structurally by scanning electron microscopy; for a distinct identification of the interface region and analysing the degree of cross-interface diffusion, the isothermal entropy change was measured by a vibrating sample magnetometer as the magnetic transition temperature (Curie temperature) is very sensitive to the dopant level in ceramics. Also the purpose of developing this graded ceramic tape casting was applications of these specific magnetocaloric properties within the magnetic refrigeration technology.

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Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials, Imaging and Structural Analysis
Contributors: Bulatova, R., Bahl, C., Andersen, K. B., Kuhn, L. T., Pryds, N.
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Volume: 12
Issue number: 4
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Highly Confined Electronic and Ionic Conduction in Oxide Heterostructures

The conductance confined at the interface of complex oxide heterostructures provides new opportunities to explore nanoelectronic as well as nanionic devices. In this talk I will present our recent results both on ionic and electronic conductivity at different heterostructures systems. In the first part of my talk I will show some of our resent results that we demonstrated the possibility of stabilizing δ-Bi2O3 using highly coherent interfaces of alternating layers. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for Bi2O3-based materials, is achieved[1]. These confined heterostructures provide a playground not only for new high ionic conductivity phenomena that are sufficiently stable but also uncover a large variety of possible technological perspectives.


General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Pryds, N.
Number of pages: 1
High performance p-type segmented leg of misfit-layered cobaltite and half-Heusler alloy

In this study, a segmented p-type leg of doped misfit-layered cobaltite $\text{Ca}_{2.8}\text{Lu}_{0.15}\text{Ag}_{0.05}\text{Co}_4\text{O}_{9+\delta}$ and half-Heusler $\text{Ti}_{0.3}\text{Zr}_{0.35}\text{Hf}_{0.35}\text{CoSb}_{0.8}\text{Sn}_{0.2}$ alloy was fabricated and characterized. The thermoelectric properties of single components, segmented leg, and the electrical contact resistance of the joint part were measured as a function of temperature. The output power generation characteristics of segmented legs were characterized in air under various temperature gradients, $\Delta T$, with the hot side temperature up to 1153 K. At $\Delta T \approx 756$ K, the maximum conversion efficiency reached a value of $\sim 5\%$, which is about 65% of that expected from the materials without parasitic losses. The long-term stability investigation for two weeks at the hot and cold side temperatures of 1153/397 K shows that the segmented leg has good durability as a result of stable and low electrical resistance contacts.

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Contributors: Le, T. H., Van Nong, N., Snyder, G. J., Viet, M. H., Balko, B., Han, L., Stamate, E., Linderoth, S., Pryds, N.
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Web of Science (2017): Impact factor 6.377
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Web of Science (2015): Impact factor 4.801
Web of Science (2015): Indexed yes
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Web of Science (2013): Impact factor 3.59
An enhanced thermal stability in thermoelectric Ca₃Co₄O₉ thin films up to 550 °C in an oxygen rich environment was demonstrated by high-temperature electrical and X-ray diffraction measurements. In contrast to generally performed heating in helium gas, it is shown that an oxygen/helium mixture provides sufficient thermal contact, while preventing the previously disregarded formation of oxygen vacancies. Combining thermal cycling with electrical measurements proves to be a powerful tool to study the real intrinsic thermoelectric behaviour of oxide thin films at elevated temperatures. © 2015 AIP Publishing LLC.
Hybrid TEG-heat exchanger module for electrical power production

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Modeling constrained sintering of bi-layered tubular structures

Constrained sintering of tubular bi-layered structures is being used in the development of various technologies. Densification mismatch between the layers making the tubular bi-layer can generate stresses, which may create processing defects. An analytical model is presented to describe the densification and stress developments during sintering of tubular bi-layered samples. The correspondence between linear elastic and linear viscous theories is used as a basis for derivation of the model. The developed model is first verified by finite element simulation for sintering of tubular bi-layer system. Furthermore, the model is validated using densification results from sintering of bi-layered tubular ceramic oxygen membrane based on porous MgO and Ce0.9Gd0.1O1.95-d layers. Model input parameters, such as the shrinkage kinetics and viscous parameters are obtained experimentally using optical dilatometry and thermo-mechanical analysis. Results from the analytical model are found to agree well with finite element simulations as well as measurements from sintering experiment.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Electrofunctional materials, San Diego State University
Modeling the Microstructural Evolution During Constrained Sintering

A numerical model able to simulate solid-state constrained sintering is presented. The model couples an existing kinetic Monte Carlo model for free sintering with a finite element model (FEM) for calculating stresses on a microstructural level. The microstructural response to the local stress as well as the FEM calculation of the stress field from the microstructural evolution is discussed. The sintering behavior of a sample constrained by a rigid substrate is simulated. The constrained sintering results in a larger number of pores near the substrate, as well as anisotropic sintering shrinkage, with significantly enhanced strain in the central upper part of the sample surface, and minimal strain at the edges near the substrate. All these features have also previously been observed experimentally.
Thin films solar cells based on Cu2ZnSnS4 (CZTS) as absorber layer have seen a rapid development leading to a world record of 8.8% [1]. However, other p-type semiconductors with fewer elements and reduced complexity compared to CZTS are also available, such as ternary Cu–Sn–S systems, i.e. Cu2SnS3 (CTS) [2].
Numerical simulation of viscoelastic free-surface flows using a streamfunction/log-conformation formulation and the volume-of-fluid method

This thesis presents a new numerical algorithm for the simulation of two-dimensional multiphase viscoelastic flows. The simulation of viscoelastic flows has both a scientific importance and practical implications in polymer processing. This work has put the emphasis on the extrusion of polymeric materials, where viscoelastic effects cause dynamical instabilities, despite the very simple geometry. This thesis reviews the popular differential constitutive models derived from molecular theories of dilute polymer solutions, polymer networks, and entangled polymer melts, as well as the inelastic phenomenological models describing shear-thinning and viscoelastic (yield stress) fluids, based on the generalized Newtonian fluid model. In addition, the numerical issues related to the high Weissenberg number problem, and its remedy with the log-conformation representation, are discussed. The proposed algorithm utilizes a new streamfunction/log-conformation scheme. The drawbacks of the classical velocity-pressure decoupled method, which is by far the most popular approach, are remedied with the pure streamfunction formulation, which is derived from the pressureless vorticity-based methods. The implicit pure streamfunction formulation is formally more accurate than the velocity-pressure decoupled method, because it is immune of decoupling errors. Moreover, the absence of decoupling enhances the stability of the calculation. The governing equations (conservation laws and constitutive models) are discretized with the finite-volume method, on a Cartesian grid. Discrete curl operators are applied to the discretized momentum equations in order to obtain the matrix system of the discrete streamfunction variables. The coupling of the streamfunction/log-conformation scheme with adaptive under-relaxation and adaptive time-stepping yield a robust and efficient viscoelastic flow solver algorithm. The potential extension of the method to three-dimensional simulations is also discussed in this thesis. Bi-phasic/free-surface flows are modelled with the Volume-of-Fluid (VOF) method, and the standard piecewise-linear-interface-construction technique. In addition, a new Cellwise Conservative Unsplit (CCU) advection scheme is presented. The CCU scheme updates the liquid volume fractions based on cellwise backward-tracking of the liquid volumes. The algorithm calculates non-overlapping and conforming adjacent donating regions, which ensures the boundedness and conservativeness of the liquid volume. As a result, the CCU advection scheme is overall more accurate in classical benchmark tests, than the other state-of-the-art multidimensional VOF-advection schemes. In complex flows, the convergence rate of the CCU scheme with mesh refinements is between 2 and 3. Moreover, the remaining geometrical errors are mostly due to the inability of the standard piecewise linear interface to represent subgrid material topologies (i.e. high curvatures and thin material filaments), rather than the proposed CCU advection scheme. This thesis reports examples of numerical simulations of the Oldroyd-B liquid, calculated with the proposed streamfunction/log-conformation/VOF-CCU methodology, implemented in Matlab. A thorough investigation of the viscoelastic flow in the lid-driven cavity is conducted. The streamfunction/log-conformation shows second-order accuracy and numerical stability at very large time-step increments, which demonstrates the robustness of the scheme. The numerical results at moderate Weissenberg numbers are in good agreement with the literature. Moreover, the enhancement of numerical stability, with the streamfunction/log-conformation scheme, makes it possible to simulate elastic instabilities at high Weissenberg numbers. Quasi-periodic elastic instabilities at the upstream corner appear to be a mechanism that dissipates the stored elastic energy. The simulations of viscoelastic flows in the planar 4:1 contraction are also in good agreement with data in the literature. Finally, preliminary simulations of extrudate swelling show that the fracture melt extrusion defect could be caused by instabilities in the stress layer at the surface of the die, triggered at moderate Weissenberg numbers.
Optimization of spark plasma sintering conditions for antimony-doped bismuth telluride

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, Fraunhofer Institute for Material and Beam Technology
Contributors: Han, L., Van Nong, N., Le, T. H., Pham, H. N., Hegelund Spangsdorf, S., Roch, A., Stepien, L., Pryds, N.
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Optimization of the Mechanical and Electrical Performance of a Thermoelectric Module
Finite element (FE) simulation of a thermoelectric (TE) module was conducted to optimize its geometrical dimensions in terms of mechanical reliability and performance. The TE module consisted of bismuth telluride, nand p-type legs. The geometrical dimensions of the module, i.e. leg length and leg cross-sectional area, were varied and the corresponding maximum thermal stress, output power and efficiency of the module was obtained. The optimal design of the module was then suggested based on minimizing the thermal stresses and maximizing the performance, i.e. power and efficiency. The optimal dimensions at a maximum von Mises stress of 75 MPa was a leg length of 2-2.5 mm, a leg width of 1.5-2 mm, which resulted in an efficiency of 7.2. Finally, the influence of solders, i.e. solder material between the leg, the interconnector and the top ceramic layer, on the induced thermal stresses and the module performance was investigated. The results revealed that transition from elastic to plastic deformation in the solder decreases the induced thermal stresses significantly. Moreover, beyond the elastic limit the stress magnitude is very much dependent on the magnitude and mechanism of the plastic deformation in the module. The present study provides a basis for unique and new optimization scheme of the TE modules in terms of endurance and performance.

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BFI (2016): BFI-level 1
Oxide interfaces provide an opportunity for electronics. However, patterning of electron gases at complex oxide interfaces is challenging. In particular, patterning of complex oxides while preserving a high electron mobility remains underexplored and inhibits the study of quantum mechanical effects where extended electron mean free paths are paramount. This letter presents an effective patterning strategy of both the amorphous-LaAlO$_3$/SrTiO$_3$ (a-LAO/STO) and modulation-doped
amorphous-LaAlO$_3$/La$_{7/8}$Sr$_{1/8}$MnO$_3$/SrTiO$_3$ (a-LAO/LSM/STO) oxide interfaces. Our patterning is based on selective wet etching of amorphous-LSM (a-LSM) thin films, which acts as a hard mask during subsequent depositions. Strikingly, the patterned modulation-doped interface shows electron mobilities up to $\sim$8 700 cm$^2$/V s at 2 K, which is among the highest reported values for patterned conducting complex oxide interfaces that usually are $\sim$1 000 cm$^2$/V s at 2K. © 2015 AIP Publishing LLC.
Patterning of high-mobility.pdf

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Bibliographical note

Percolative nature of A-site disordered La$_{0.75}$Ca$_{0.25}$-xSr$_x$MnO$_3$ manganites

Magnetic, resistive, and magnetoresistance measurements were used to investigate the percolative nature of A-site disordered La$_{0.75}$Ca$_{0.25}$xSr$_x$MnO$_3$ (x = 0, 0.10) manganites. La$_{0.75}$Ca$_{0.25}$Sr$_{0.10}$MnO$_3$ has an orthorhombic structure and second order magnetic phase transition indicates the presence of two prominent downturns $T^*$ and $T_{ferro}$ above the Curie temperature ($T_C$) in the derivative of the inverse susceptibility measurements. These observations are in agreement with the percolation model and the results are discussed in the light of phase separation happening in small polarons present in the insulating phase. © 2015 Elsevier B.V. All rights reserved.

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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.14 SJR 0.651 SNIP 0.918
Web of Science (2016): Impact factor 2.084
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.32 SJR 0.692 SNIP 0.989
Web of Science (2015): Impact factor 2.101
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.59 SJR 0.847 SNIP 1.281
Web of Science (2014): Impact factor 2.259
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.38 SJR 0.813 SNIP 1.254
Web of Science (2013): Impact factor 2.129
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.41 SJR 0.912 SNIP 1.434
Web of Science (2012): Impact factor 2.072
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.048 SNIP 1.267
Web of Science (2010): Impact factor 2.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.983 SNIP 1.292
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.929 SNIP 1.302
Scopus rating (2007): SJR 1.001 SNIP 1.332
Scopus rating (2006): SJR 0.955 SNIP 1.336
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.799 SNIP 1.188
Scopus rating (2004): SJR 0.676 SNIP 0.929
Scopus rating (2003): SJR 0.644 SNIP 1.123
Scopus rating (2002): SJR 0.609 SNIP 0.785
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Pulsed laser deposition from ZnS and Cu$_2$SnS$_3$ multicomponent targets

Thin films of ZnS and Cu$_2$SnS$_3$ have been produced by pulsed laser deposition (PLD), the latter for the first time. The effect of fluence and deposition temperature on the structure and the transmission spectrum as well as the deposition rate has been investigated, as has the stoichiometry of the films transferred from target to substrate. Elemental analysis by energy dispersive X-ray spectroscopy indicates lower Sn and Sn content in Cu$_2$SnS$_3$ films produced at higher fluence, whereas this trend is not seen in ZnS. The deposition rate of the compound materials measured in atoms per pulse is considerably larger than that of the individual metals, Zn, Cu, and Sn.

General information
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Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
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ISI indexed (2013): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
Segmentation of low-cost high efficiency oxide-based thermoelectric materials

Thermoelectric (TE) oxide materials have attracted great interest in advanced renewable energy research owing to the fact that they consist of abundant elements, can be manufactured by low-cost processing, sustain high temperatures, be robust and provide long lifetime. However, the low conversion efficiency of TE oxides has been a major drawback limiting these materials to broaden applications. In this work, theoretical calculations are used to predict how segmentation of oxide and semimetal materials, utilizing the benefits of both types of materials, can provide high efficiency, high temperature oxide-based segmented legs. The materials for segmentation are selected by their compatibility factors and their conversion efficiency versus material cost, i.e., "efficiency ratio". Numerical modelling results showed that conversion efficiency could reach values of more than 10% for unicouples using segmented legs based p-type Ca3Co4O9 and n-type ZnO oxides excluding electrical and thermal losses. It is found that the maximum efficiency of segmented unicouple could be linearly decreased with increasing the interfacial contact resistance. The obtained results provide useful tool for designing a low-cost and high efficiency thermoelectric modules based-oxide materials.
Segmented Thermoelectric Oxide-Based Module for High-Temperature Waste Heat Harvesting

We report a high-performance thermoelectric (TE) oxide-based module using the segmentation of half-Heusler $\text{Ti}_{0.35}\text{Zr}_{0.35}\text{Hf}_{0.35}\text{CoSb}_{0.8}\text{Sn}_{0.2}$ and misfit-layered cobaltite $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ as the p-leg and 2% Al-doped ZnO as the n-leg. The maximum output power of a 4-couple segmented module at $\Delta T=700$ K attains a value of approximately 6.5 kWm$^{-2}$, which is three times higher than that of the best reported non-segmented oxide module. The TE properties of individual legs, as well as the interfacial contact resistances, were characterized as a function of temperature. Numerical modeling was used...
to predict the efficiency and to evaluate the influence of the electrical and thermal losses on the performance of TE modules. Initial long-term stability tests of the module at the hot and the cold side temperatures of 1073 K and 444 K, respectively, showed a promising result with 4% degradation for 48 h operating in air.

**General information**

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Johannes Gutenberg University, California Institute of Technology
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Web of Science (2015): Impact factor 2.557
Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
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Solid-oxide fuel cells

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Stabilized thin film heterostructure for electrochemical applications.
The invention provides a method for the formation of a thin film multi-layered heterostructure upon a substrate, said method comprising the steps of: a. providing a substrate; b. depositing a buffer layer upon said substrate, said buffer layer being a layer of stable ionic conductor (B); c. depositing a layer A upon said buffer layer, said layer A being a layer of fast ionic conductor (A), said layer A having a thickness (tA) of 20 nm or less; d. depositing a layer B upon said layer A, said layer B being a layer of stable ionic conductor (B), said layer B having a thickness (tB) of 150 nm or less; and e. repeating steps b. and c. a total of N times, such that N repeating pairs of layers (A/B) are built up, wherein N is 1 or more. The invention also provides a thin film multi-layered heterostructure as such, and the combination of a thin film multi-layered heterostructure and a substrate. The heterostructure finds use as an electroceramic, in particular in SOFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Contributors: Esposito, V., Sanna, S., Pryds, N., Linderoth, S.
Publication date: 2015

The Elastocaloric Effect: A Way to Cool Efficiently
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Composites Mechanics and Materials Mechanics, University of Barcelona
Contributors: Tusek, J., Engelbrecht, K., Millán-Solsona, R., Mañosa, L., Vives, E., Mikkelsen, L. P., Pryds, N.
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 16.78 SJR 8.23 SNIP 2.347
Web of Science (2017): Impact factor 21.875
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.515 SNIP 2.14
Web of Science (2016): Impact factor 16.721
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 14.2 SJR 6.219 SNIP 2.546
Web of Science (2015): Impact factor 15.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Thin films of CZTS prepared by Pulsed Laser Deposition

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials, Experimental Surface and Nanomaterials Physics
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Electronic versions: Andcan_MRS2015_poster_JS_JS2.pdf
Research output: Research - peer-review → Journal article – Annual report year: 2015

ZnS top layer for enhancement of the crystallinity of CZTS absorber during the annealing

Pulsed Laser Deposition (PLD) of thin films of Cu2ZnSnS4 (CZTS) has not yet led to solar cells with high efficiency. The reason for the relative low efficiency is discussed and a way to overcome this issue is presented. The present thin film absorbers of CZTS suffer from loss of volatile Zn during the plasma-assisted transfer with PLD. This can be compensated by adding a thin layer of ZnS (∼ 80 nm) on top of the CZTS layer before the annealing. In this work the stack ordering of the two layers CZTS and ZnS is investigated, indicating that the configuration with ZnS on top of a CZTS film gives a better crystalline quality of CZTS after the annealing, as demonstrated by X-ray diffraction and Raman spectroscopy.
Analysis of the internal heat losses in a thermoelectric generator

A 3D thermoelectric numerical model is used to investigate different internal heat loss mechanisms for a thermoelectric generator with bismuth telluride p- and n-legs. The model considers all thermoelectric effects, temperature dependent material parameters and simultaneous convective, conductive and radiative heat losses, including surface to surface radiation. For radiative heat losses it is shown that for the temperatures considered here, surface to ambient radiation is a good approximation of the heat loss. For conductive heat transfer the module efficiency is shown to be comparable to the case of radiative losses. Finally, heat losses due to internal natural convection in the module is shown to be negligible for the millimetre sized modules considered here. The combined case of radiative and conductive heat transfer resulted in the lowest efficiency. The optimized load resistance is found to decrease for increased heat loss. The leg dimensions are varied for all heat losses cases and it is shown that the ideal way to construct a TEG module with minimal heat losses and maximum efficiency is to either use a good insulating material between the legs or evacuate the module completely, and use small and wide legs closely spaced. (C) 2014 Elsevier Masson SAS. All rights reserved.
Characterization of the interface between an Fe–Cr alloy and the p-type thermoelectric oxide Ca$_3$Co$_4$O$_9$

A customized Fe–Cr alloy that has been optimized for high temperature applications in oxidizing atmospheres has been interfaced via spark plasma sintering (SPS) with a p-type thermoelectric oxide material: calcium cobaltate (Ca$_3$Co$_4$O$_9$). The properties of the alloy have been analyzed for its compatibility with the Ca$_3$Co$_4$O$_9$ in terms of its thermal expansion and transport properties. The thermal and electrical contact resistances have been measured as a function of temperature, and the long term electronic integrity of the interface analyzed by measuring the resistance vs. time at an elevated temperature. The kinetics of the interface have been analyzed through imaging with scanning electron microscopy (SEM), elemental analysis using energy dispersive spectroscopy (EDS), and phase identification with X-ray diffraction (XRD). The results reveal the formation of an intermediate phase containing calcium and chromium in the interface that is highly resistive at room temperature, but conducting at the intended thermoelectric device hot-side operating temperature of 800 °C. As the alloy is well matched in terms of its thermal expansion and highly conducting compared to the Ca$_3$Co$_4$O$_9$, it may be further considered as an interconnect material candidate at least with application on the hot-side of an oxide thermoelectric power generation module.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Aarhus University
Contributors: Holgate, T., Han, L., Wu, N., Bejøsen, E. D., Christensen, M., Iversen, B. B., Van Nong, N., Pryds, N.
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Publication information
Journal: Journal of Alloys and Compounds
Volume: 582
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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
Web of Science (2015): Impact factor 3.014
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.13 SJR 1.117 SNIP 1.632
Web of Science (2014): Impact factor 2.999
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.73 SJR 1.059 SNIP 1.583
Web of Science (2013): Impact factor 2.726
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.43 SJR 1.246 SNIP 1.57
Web of Science (2012): Impact factor 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.41 SJR 1.164 SNIP 1.463
Web of Science (2011): Impact factor 2.289
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
Web of Science (2010): Impact factor 2.138
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.956 SNIP 1.372
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
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
Scopus rating (2005): SJR 1.088 SNIP 1.208
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.922 SNIP 1.354
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.949 SNIP 1.051
Scopus rating (2002): SJR 0.733 SNIP 1.063
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.634 SNIP 0.966
Densification of Highly Defective Ceria by High Temperature Controlled Re-Oxidation

Highly enhanced densification and grain growth of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-\delta}$ (CGO, gadolinium-doped ceria, with 10 mol% Gd) is achieved in low oxygen activity atmospheres. However, the material can suffer mechanical failures during cooling when the re-oxidation process is not controlled due to the large volume changes. In this work, the redox process of CGO is investigated using dilatometry, microscopy, electrochemical impedance spectroscopy and thermodynamic analysis. In addition, the conditions allowing controlled re-oxidation and cooling in order to preserve the mechanical integrity of the CGO component are defined: this can be achieved over a wide temperature range (800–1200 °C) by gradually increasing the oxygen content of the atmosphere. It is found that the electrical conductivity of the CGO, particularly at low temperature (<450 °C) is influenced by the sintering and controlled re-oxidation conditions. An increase in activation energy for conduction at low temperature is observed as the re-oxidation temperature decreases. Moreover it was observed that the ionic conductivity blocking effect, usually associated with grain boundary contributions, is not influenced by the grain size but rather by the chemical history of the material. © 2014 The Electrochemical Society.

General information
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Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Ceramic Engineering & Science
Contributors: Ni, D. W., Glasscock, J., Pons, A., Zhang, W., Prasad, A., Sanna, S., Pryds, N., Esposito, V.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Impact factor 3.662
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Impact factor 3.259
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.17 SJR 1.115 SNIP 1.066
Web of Science (2015): Impact factor 3.014
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.36 SJR 1.213 SNIP 1.25
Web of Science (2014): Impact factor 3.266
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Design and initial testing of a compact and efficient rotary AMR prototype

MAGGIE, a new AMR prototype, is presented. It has been designed to produce a temperature span and cooling power relevant to commercial refrigeration applications combined with an attractive COP and a compact design. Concepts and design considerations are described. Initial non optimized tests show a COP of 3.6 at a temperature span of 7.2K with 103 W of cooling power.

General information
Design of thermoelectric modules for both mechanical reliability and performance using FE simulation

Thermo-mechanical modeling of the TE modules provides an efficient tool for assessing the mechanical strength of the modules against the induced thermal stresses and subsequently optimizing them in terms of the mechanical reliability. However, the design of TE modules in terms of mechanical reliability cannot be separated completely from the design for performance. These two objectives may conflict such that the improvement of the design parameters for one objective can deteriorate the other one. This trade off can be seen particularly when the geometrical dimensions of a TE module is optimized for these two objectives.

The current study deals with FE simulation of the TE modules to optimize their geometrical dimension in terms of mechanical reliability and performance. First, FE simulation of a TE module consisting of bismuth telluride alloys is carried out and the induced thermal stresses, output power and efficiency of the module is calculated. Then, the geometrical dimensions of the module including the leg length and the cross sections of the TE elements are varied and the corresponding maximum thermal stresses, output power and efficiency of the modules are obtained. Based on the results, the geometrical dimensions of the TE elements for both mechanical reliability and performance are optimized to obtain a compromise design. The present work provides a basis for optimizing the TE modules in terms of their life time and performance.

Development and experimental results from a 1 kW prototype AMR

A novel rotary magnetic refrigeration device has been designed and constructed following the concepts recently outlined in Bahl et al. (2011). The magnet and flow system design allow for almost continuous usage of both the magnetic field and the magnetocaloric material in 24 cassettes, each containing an active magnetic regenerator (AMR) bed. The prototype design facilitates easy exchange of the 24 cassettes, allowing the testing of different material amounts and compositions. Operating with 2.8 kg of commercial grade Gd spheres a maximum no-span cooling power of 1010 W and a maximum zero load temperature span of 25.4 K have been achieved. For the purpose of actual operation, simultaneous high span and high performance is required. At a heat load of 200 W a high temperature span of 18.9 K has been obtained, dropping to a span of 13.8 K at the higher heat load value of 400 W.
Development and Processing of p-type Oxide Thermoelectric Materials

The main aim of this research is to investigate and develop well-performing p-type thermoelectric oxide materials that are sufficiently stable at high temperatures for power generating applications involving industrial processes. Presently, the challenges facing the widespread implementation of thermoelectric power generation technology lie in the high cost and low efficiency of thermoelectric systems. Scalable and practical applications, including commercialization based on the currently used materials are subject to environmental and cost issues, and thus are difficult to be realized. Metal oxides have attracted much attention due to features such as a natural abundance of constituent elements, environmental benignity and durability at high temperature in air. This research aims to develop and investigate the misfit-layered cobaltate Ca₃Co₄O₉+δ, which demonstrates a large potential for high temperature applications owing to its large positive Seebeck coefficient (S) together with a metallic-like electrical conductivity and a low thermal conductivity typical of a "phonon glass–electron crystal". The research begins with the study of Ca₃Co₄O₉+δ syntheses by solid-state and sol–gel reactions, followed by the use of spark plasma sintering (SPS) processing with different conditions such as sintering temperatures, applied pressures and ramping rates. With characterization of the microstructure, bulk density and thermoelectric transport properties, Ca₃Co₄O₉+δ synthesized by sol–gel reaction followed by the proper spark plasma sintering processing conditions is suggested to be a beneficial means of obtaining high-performance Ca₃Co₄O₉+δ owing to the resulting smaller particle sizes and enhanced grain alignment. Other than the conventional solid-state reaction and sol–gel methods, a rapid auto-combustion reaction for the synthesis of Ca₃Co₄O₉+δ nano-powder is developed to realize nanostructuring for enhanced thermoelectric properties. The procedure is a modification of the conventional citrate–nitrate sol–gel method where an auto-combustion process is initiated by a controlled thermal oxidation–reduction reaction. This synthesis produces morphological and compositional homogeneity, and fine, well-defined particle sizes. With determined optimal spark plasma sintering processing conditions, highly dense and beneficially textured Ca₃Co₄O₉+δ can be fabricated. Introducing extrinsic elements as dopants may exert great influence on the thermoelectric properties. Singly Fe-doped and Fe/Y co-doped Ca₃Co₄O₉+δ samples synthesized by the newly developed auto-combustion reaction followed by spark plasma sintering processing with the effects of Fe and Fe/Y doping on the high temperature thermoelectric properties (from room temperature to 800 °C) were investigated and discussed. The Fe substitution at the Co-sites effectively reduces the electrical resistivity (ρ) while the Seebeck coefficient is influenced only slightly. Y substitution for Ca₂⁺ leads to an increase in the Seebeck coefficient but also in the electrical resistivity. With a proper amount of Fe co-doping, the increase in the electrical resistivity was compensated, and together with the improved Seebeck coefficient the addition of Fe lead to the enhancement of the overall thermoelectric performance. With the aforementioned approach, further investigation has been conducted on rare-earth doping with Ce in Ca₃Co₄O₉+δ in order to explore the effects on the high temperature thermoelectric properties. With the auto-combustion reaction synthesis followed by spark plasma sintering processing, Ca₃-xCexCo₄O₉+δ exhibited increasing electrical resistivity and Seebeck coefficient with increasing Ce doping content over the whole measured temperature range, while the in-plane thermal conductivity (κ) was only slightly influenced. Since the introduction of Ce leads to a small decrease in the power factor (PF) but also reduction in the thermal conductivity resulting in the figure-of-merit (ZT) values being similar to the un-doped Ca₃Co₄O₉+δ, the ZT may be enhanced in rare-earth and transition metal (e.g., Ce and Fe) co-doped Ca₃Co₄O₉+δ through decoupling of the otherwise interdependent electronic and thermal transport properties.

General information

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Wu, N., Linderoth, S., Pryds, N., Van Nong, N.
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Effects of conducting oxide barrier layers on the stability of Crofer® 22 APU/Ca₃Co₄O₉⁺δ interfaces

Practical implementation of oxide thermoelectrics on an industrial or commercial scale for waste heat energy conversion requires the development of chemically stable interfaces between metal interconnects and oxide thermoelements that exhibit low electrical contact resistances. A commercially available high-chrome iron alloy (i.e., Crofer® 22 APU) serving
as the interconnect metal was spray coated with LaNi$_{0.6}$Fe$_{0.4}$O$_{3}$ (LNFO) or (Mn,Co)$_3$O$_4$ spinel and then interfaced with a p-type thermoelectric material—calcium cobaltate (Ca$_3$Co$_4$O$_9$)—using spark plasma sintering. The interfaces have been characterized in terms of their thermal and electronic transport properties and chemical stability. With long-term exposure of the interfaced samples to 800 °C in air, the cobalt–manganese spinel acted as a diffusion barrier between the Ca$_3$Co$_4$O$_9$ and the Crofer® 22 APU alloy resulting in improved interfacial stability compared to that of samples containing LNFO as a barrier layer, and especially those without any barrier. The initial area specific interfacial resistance of the Ca$_3$Co$_4$O$_9$/((Mn,Co)$_3$O$_4$/Crofer® 22 APU interface at 800 °C was found to be ∼1 mΩ·cm$^2$.

General information
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Contributors: Holgate, T. C., Han, L., Wu, N., Van Nong, N., Pryds, N.
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Journal: Journal of Materials Research
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.55 SJR 0.61 SNIP 0.661
Web of Science (2017): Impact factor 1.495
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.51 SJR 0.651 SNIP 0.664
Web of Science (2016): Impact factor 1.673
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.48 SJR 0.638 SNIP 0.718
Web of Science (2015): Impact factor 1.579
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.8 SJR 0.811 SNIP 0.948
Web of Science (2014): Impact factor 1.647
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.77 SJR 0.832 SNIP 0.835
Web of Science (2013): Impact factor 1.815
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.57 SJR 0.92 SNIP 0.985
Web of Science (2012): Impact factor 1.713
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.49 SJR 0.877 SNIP 0.841
Web of Science (2011): Impact factor 1.434
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.043 SNIP 0.873
Web of Science (2010): Impact factor 1.402
Web of Science (2010): Indexed yes
Effects of morphology on the thermoelectric properties of Al-doped ZnO

The nanoparticles of Al-doped ZnO were successfully grown into rod-like and platelet-like morphologies by soft chemical routes. These powders were consolidated using spark plasma sintering (SPS) technique. The samples consolidated from rods and platelets exhibited characteristic structures with preferential orientation while the sample consolidated from nanoparticles did not show any sign of preferential orientation. The measured ZT values along the preferred orientation directions were found to be 0.16 and 0.25 at 1223 K for the samples consolidated from rods and platelets, respectively. The sample consolidated from nanoparticles exhibited fine grains and highly distributed nanoprecipitates, resulting in a ZT value of 0.3 at 1223 K due to the lower thermal conductivity resulting from nanostructuring. Using the simple parabolic band model and Debye–Callaway thermal transport model, the anisotropic properties of the nanostructured samples were elucidated and the influence of the grain size and nanoprecipitates on the electron and phonon transport was analyzed and discussed in detail.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Kyushu University
Contributors: Han, L., Van Nong, N., Zhang, W., Le, T. H., Holgate, T., Tashiro, K., Ohtaki, M., Pryds, N., Linderoth, S.
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Publication information
Journal: R S C Advances
Volume: 4
ISSN (Print): 2046-2069
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736
Web of Science (2017): Impact factor 2.936
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Web of Science (2016): Impact factor 3.108
Web of Science (2016): Indexed yes
Experimental results for a recently developed prototype magnetic refrigeration device at the Technical University of Denmark (DTU) were obtained and compared with numerical simulation results. A continuously rotating active magnetic regenerator (AMR) using 2.8 kg packed sphere regenerators of gadolinium (Gd) was employed. With operating frequencies up to 10 Hz and volumetric flow rates up to 600 L h⁻¹, the prototype has shown high performance and the results are consistent with predictions from numerical modelling. Magnetocaloric properties of the Gd spheres were obtained experimentally and implemented in a one-dimensional numerical AMR model that includes also the parasitic losses from the prototype. The temperature span for a thermal load of 200 W as a function of frequency was measured and modelled. Moreover, the temperature span dependence on the cooling capacity as a function of cycle frequency was determined. A detailed study of these parasitic losses was carried out experimentally and numerically.

General information
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Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Federal University of Santa Catarina
Contributors: Lozano, J., Engelbrecht, K., Bahl, C. R., Nielsen, K. K., Barbosa, J. J., Prata, A., Pryds, N.
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ISSN (Print): 0140-7007
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.46 SJR 1.471 SNIP 1.888
Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Finite element modeling of camber evolution during sintering of bi-layers

The need for understanding the mechanisms and optimization of shape distortions during sintering of bilayers is necessary while producing structures with functionally graded architectures. A finite element model based on the continuum theory of sintering was developed to understand the camber developments during sintering of bilayers composed of La0.85Sr0.15MnO3 and Ce0.9Gd0.1O1.95 tapes. Free shrinkage kinetics of both tapes were used to estimate the parameters necessary for the finite element models. Systematic investigations of the factors affecting the kinetics of distortions such as gravity and friction as well as the initial geometric parameters of the bilayers were made using optical dilatometry experiments and the model. The developed models were able to capture the observed behaviors of the bilayers’ distortions during sintering. Finally, we present the importance of understanding and hence making use of the effect of gravity and friction to minimize the shape distortions during sintering of bilayers.

General information
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Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Electrofunctional materials
Contributors: Tadesse Molla, T., Ni, D. W., Bulatova, R., Bjørk, R., Bahl, C. R., Pryds, N., Frandsen, H. L.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.06 SJR 0.95 SNIP 1.325
Web of Science (2017): Impact factor 2.956
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1.028 SNIP 1.428
Web of Science (2016): Impact factor 2.841
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.71 SJR 0.995 SNIP 1.37
Web of Science (2015): Impact factor 2.787
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.78 SJR 1.167 SNIP 1.595
Web of Science (2014): Impact factor 2.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.52 SJR 1.16 SNIP 1.48
Web of Science (2013): Impact factor 2.428
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.39 SJR 1.271 SNIP 1.5
Web of Science (2012): Impact factor 2.107
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.45 SJR 0.958 SNIP 1.447
Web of Science (2011): Impact factor 2.272
ISI indexed (2011): ISI indexed yes
A rapid method for the synthesis of Ca$_3$Co$_4$O$_{9+\delta}$ powder is introduced. The procedure is a modification of the conventional citric-nitrate sol–gel method where an auto-combustion process is initiated by a controlled thermal oxidation–reduction reaction. The resulting powders inherit the advantages of a wet chemical synthesis, such as morphological and compositional homogeneity, and fine, well-defined particle sizes coming from the controlled nature of the auto-combustion. Optimized spark plasma sintering (SPS) processing conditions were determined and used to fabricate dense and highly c-axis oriented samples. The microstructure and thermoelectric transport properties were determined both parallel ($\parallel$) and perpendicular ($\perp$) to the SPS pressure axis in order to investigate any possible anisotropy variations in the transport properties. At 800°C, power factors of 506 μW/m K² ($\perp$) and 147 μW/m K² ($\parallel$), thermal conductivities values of 2.53 W/m K ($\perp$) and 1.25 W/m K ($\parallel$), and resulting figures-of-merit, ZT, of 0.21 ($\perp$) and 0.13 ($\parallel$) were observed. © 2013 Elsevier Ltd. All rights reserved.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Impact factor 3.794
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Impact factor 3.454
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.03 SJR 1.135 SNIP 1.817
Web of Science (2015): Impact factor 2.933
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.16 SJR 1.163 SNIP 2.083
Web of Science (2014): Impact factor 2.947
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BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.81 SJR 1.293 SNIP 2.207
Web of Science (2012): Impact factor 2.36
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.83 SJR 1.343 SNIP 2.195
Web of Science (2011): Impact factor 2.353
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.383 SNIP 1.93
Web of Science (2010): Impact factor 2.575
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.374 SNIP 1.712
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BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.139 SNIP 1.627
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.212 SNIP 1.745
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.22 SNIP 1.665
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.095 SNIP 1.633
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.055 SNIP 1.743
Scopus rating (2003): SJR 1.151 SNIP 1.496
Scopus rating (2002): SJR 1.101 SNIP 1.184
High Temperature Thermoelectric Properties of ZnO Based Materials

This thesis investigated the high temperature thermoelectric properties of ZnO based materials. The investigation first focused on the doping mechanisms of Al-doped ZnO, and then the influence of spark plasma sintering conditions on the thermoelectric properties of Al, Ga-dually doped ZnO. Following that, the nanostructuring effect for Al-doped ZnO was systematically investigated using samples with different microstructure morphologies. At last, the newly developed ZnCdO materials with superior thermoelectric properties and thermal stability were introduced as promising substitutions for conventional ZnO materials. For Al-doped ZnO, α- and γ-Al2O3 were selectively used as dopants in order to understand the doping mechanism of each phase and their effects on the thermoelectric properties. The samples were prepared by the spark plasma sintering technique from precursors calcined at various temperatures. Clear correlations between the initial crystallographic phase of the dopants and the thermoelectric properties of the resulting Al-doped ZnO were observed. For Al, Ga-dually doped ZnO, the spark plasma sintering conditions together with the microstructural evolution and thermoelectric properties of the samples were investigated in detail. A proposed solid-state-reaction model suggested that a sintering temperature above 1223K would be preferable in order to achieve phase equilibrium in the samples. The sintering mechanism of the ZnO particles and microstructural evolutions at different sintering temperatures were investigated by the simulation of the self-Joule-heating effect of the individual particles. The effects of nanostructuring in Al-doped ZnO were systematically investigated using samples with different microstructural morphologies. The samples with preferentially oriented grains exhibited anisotropic thermoelectric properties. The measured zT values along the preferred orientation directions were found to be higher than those along the other direction. The sample consolidated from nanoparticles exhibited fine grains and widely distributed nanoprecipitates, resulting in a zT value of 0.3 at 1223 K due to the lower thermal conductivity resulting from nanostructuring. Using the simple parabolic band model and the Debye-Callaway thermal transport model, the anisotropic properties of the nanostructured samples were elucidated and the influence of the grain size and nanoprecipitates on the electron and phonon transport was analyzed and discussed in detail. In order to solve the problems of high thermal conductivity without the deterioration of electrical conductivity by nanostructuring for conventional ZnO materials, the doped ZnCdO material was proposed as a new n-type oxide thermoelectric material. The material is sintered in air in order to maintain the oxygen stoichiometry and avoid the stability issues. The successful alloying of CdO with ZnO at a molar ratio of 1:9 resulted in a significant reduction of thermal conductivity up to 7-fold at room temperature. By careful selection of the dopants and dopant concentrations, a large power factor was obtainable. The sample with the composition of Zn0.9Cd0.1Sc0.01O obtained the highest zT ~0.3 @1173 K, ~0.24 @1073K, and a good average zT which is better than the state-of-the-art n-type thermoelectric oxide materials. Meanwhile, Sc-doped ZnCdO is robust in air at high temperatures, while other n-type materials such as Al, Ga-doped ZnO will experience rapid degradation on thermoelectric performances. The thermoelectric properties of a series of samples with varied concentrations of Cd, Sc, and some other dopants are investigated and discussed in detail.

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In situ characterization of delamination and crack growth of a CGO–LSM multi-layer ceramic sample investigated by X-ray tomographic microscopy

The densification, delamination and crack growth behavior in a Ce0.9Gd0.1O1.95 (CGO) and (La0.85Sr0.15)0.9MnO3 (LSM) multi-layer ceramic sample was studied using in situ X-ray tomographic microscopy (microtomography) to investigate the critical dynamics of crack propagation and delamination in a multilayered sample. Naturally occurring defects, caused by the sample preparation process, are shown not to be critical in sample degradation. Instead defects are nucleated during the debinding step. Crack growth is significantly faster along the material layers than perpendicular to
them, and crack growth and delamination only accelerates when sintering occurs.

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Web of Science (2014): Impact factor 2.947
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
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Scopus rating (2010): SJR 1.383 SNIP 1.93
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.374 SNIP 1.712
Investigation of electronic phase segregation in $\text{La}_0.75\text{Ca}_{0.25-x}\text{Sr}_x\text{MnO}_3$ manganite

The effect of electronic phase segregation in a broad metal-insulator transition (MIT) observed in $\text{La}_{0.75}\text{Ca}_{0.25-x}\text{Sr}_x\text{MnO}_3$ ($x=0.1$) composition is investigated using heat capacity, magnetization, electrical resistivity and magnetoresistance measurements. The negative magnetoresistance of 65% in an applied magnetic field of 12T and 15% in 1T with a broad working range of 18K around 300K which is beneficial for room temperature colossal magnetoresistance (CMR) applications. The broad transition in temperature dependent zero field resistivity measurement is analyzed in the light of percolation model indicates the abundance of insulating/metallic clusters in metallic/insulating region. A significant difference between the metallic fraction around the MIT and the ferromagnetic phases observed around the Curie temperature demonstrates the interplay between volume of itinerant and polaronic electronic phases.

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Modeling Macroscopic Shape Distortions during Sintering of Multi-layers

Ceramic multi-layered composites are being used as components in various technologies ranging from electronics to energy conversion devices. Thus, different architectures of multi-layers involving ceramic materials are often required to be produced by powder processing, followed by sintering (firing). However, unintended features like shape instabilities of samples, cracks or delamination of layers may arise during sintering of multi-layer composites. Among these defects, macroscopic shape distortions in the samples can cause problems in the assembly or performance of the final component, which could result in product rejection. It is generally recognized that macroscopic shape distortion is linked to the sintering kinetics mismatch between the layer materials making the multi-layer during the co-firing process. However, there is still a need for better understanding of the deformational mechanisms with the application of flexible modeling techniques taking into account the various factors during co-firing. In addition, realistic microstructures in time/temperature need to be considered while defining the deformational behaviors of the sintering body in order to improve the predictive capabilities of the existing constitutive models. In this context, a simulation method or framework has been developed, which involves the use of sintering experiments, analytical and numerical methods. In addition to the intrinsic material parameters (shrinkage and viscous behaviors), the effect of extrinsic factors such as gravity, friction and geometry of the sample on the evolution of shape of multi-layers have been investigated. Furthermore, a new type of modeling procedure with a potential to introduce the realistic microstructure of a porous body, while defining the intrinsic material parameters,
has been developed. The linear version of the Skorohod Olevsky Viscous Sintering (SOVS) model has been used in the developed simulation models. A combination of free shrinkage rate measurements from optical dilatometry and analytical models has been used to determine the necessary input parameters for simulation of sintering of multi-layer components. Validation of the input parameters has been made indirectly by comparing model predictions for sintering of a bi-layer with measurements thereof. Moreover, a ‘master sintering curve’-type model of bi-layer sintering has been derived. This model excels in requiring a single optical dilatometry run to collect all the necessary input parameters for modeling of the sintering of the bi-layers. The determined input parameters have also been used in a finite element model, which is developed based on the continuum theory of sintering, to model the camber development during co-firing.

The effect of extrinsic factors (e.g. gravity, thickness ratio and friction) on the shape evolution of bi-layers during co-firing has been studied using the developed model and experiments. Furthermore, a new analytical model describing stresses during sintering of tubular bi-layer structures has been developed by using the direct correspondence between elasticity and linear viscous problems. The finite element model developed in this study and sintering experiments of tubular bi-layer sample have been used to verify and validate the developed analytical model for tubular bi-layered structures. A multi-scale model of shape distortions during co-firing has also been developed by coupling a meso-scale model of sintering based on kinetic Monte Carlo (kMC) methods and a macro-scale continuum model. In this case, computational homogenization theories were used to extract the viscous parameters from a representative volume element (RVE) of the porous body. The RVE was based on the microstructure obtained from the kMC model. Results from the developed analytical as well as numerical models agree well with experimental measurements of densification and camber evolutions during co-firing of bi-layers. Optimizations of the co-firing process by controlling the initial geometry of the sample and structural characteristics are also suggested. Furthermore, the multi-scale model has also shown the expected behavior of shape distortions for different bi-layers systems involving layers with the same and different sinterabilities. Based on the experimental and simulation results, the following conclusions are reached: during sintering of planar multi-layers, understanding of the effect of gravity on the camber evolution can be used in optimizing the co-sintering process so as to help achieve defect free multi-layer components. The initial thickness ratio between the layers making the multi-layer has also significant effect on the extent of camber evolution depending on the material systems. During sintering of tubular bi-layer structures, tangential (hoop) stresses are very large compared to radial stresses. The maximum value of hoop stress, which can generate processing defects such as cracks and coating peel-offs, occurs at the beginning of the sintering cycle. Unlike most of the models defining material properties based on porosity and grain size only, the multi-scale model proposed in this study has no limitation as to the number of internal parameters to define shrinkage kinetics as well as viscous properties. This feature of the model makes it to be a promising approach for extending the continuum theory of sintering.

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Modeling the microstructural evolution during constrained sintering
A mesoscale numerical model able to simulate solid state constrained sintering is presented. The model couples an existing kinetic Monte Carlo (kMC) model for free sintering with a finite element method for calculating stresses. The sintering behavior of a sample constrained by a rigid substrate is simulated, resulting in a larger number of pores near the substrate, which is also observed experimentally.

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Modelling the microstructural evolution during constrained sintering
A numerical model able to simulate solid state constrained sintering is presented. The model couples an existing kinetic Monte Carlo (kMC) model for free sintering with a finite element model (FEM) for calculating stresses on a microstructural level. The microstructural response to the local stress as well as the FEM calculation of the stress field from the microstructural evolution is discussed. The sintering behavior of a sample constrained by a rigid substrate is simulated. The constrained sintering result in a larger number of pores near the substrate, as well as anisotropic sintering shrinkage, with significantly enhanced strain in the central upper part of the sample surface, and minimal strain near the edges near the substrate. These features are also observed experimentally.

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Modelling of Tape Casting for Ceramic Applications
Functional ceramics find use in many different applications of great interest, e.g. thermal barrier coatings, piezoelectric materials, solid oxide fuel cells and electrolysis cells, membranes, and filters. It is often the case that the performance of a ceramic component can be increased markedly if it is possible to vary the relevant properties (e.g. electrical, electrochemical, or magnetic) in a controlled manner along the extent of the component. Such composites consist of different composition and/or microstructure are combined provide a new and intriguing dimension to the field of functional ceramics research. Advances in ceramic forming have enabled low cost shaping techniques such as tape casting and extrusion to be used in some of the most challenging technologies. These advances allow the design of complex components adapted to desired specific properties and applications. However, there is still only very limited insight into the processes determining the final properties of such components. Hence, the aim of the present PhD project is to obtain the required knowledge basis for the optimized processing of multi-material functional ceramics components. Recent efforts in the domain of ceramic processing are generally focused on the control of the microstructure while the importance of shaping is often underestimated. Improved performance requires the design and shaping of both controlled architectures and microstructures. Novel functionally graded ceramic materials may be formed by multilayers or adjacent grading of different ceramic materials. Such grading is often desired for optimal performance. An example is when there is a gradient in temperature or chemical environment along the component during operation; in this case the properties of each section of the component should be optimized for the local environment by grading. The grading may be between entirely different ceramic materials or merely a minor compositional alteration within one type of material. However, there are several challenges to be met for the successful fabrication of such complex structures. Rheological properties play an extremely important role for the co-processing of more than one material. Only by matching the rheological properties of the pastes, a reproducible and well defined gradient composite will be formed.

Tape casting involves the casting of a slurry onto a flat moving carrier surface. The slurry passes beneath a knife edge (doctor blade) as the carrier surface advances along a supporting table. The solvents evaporate to leave a relatively dense flexible sheet that may be stored on rolls or stripped from the carrier in a continuous process. Today, multilayers are achieved by laminating layers of different materials on top of each other. The challenge is to be able to tape cast layers of different materials simultaneously both stratified in the horizontal and in the lateral direction. Understanding how to achieve that and perfection of such a technique will open up a large variety of applications. General challenges with this process is, as mentioned, controlling the rheological properties of the slurries/pastes as they strongly affect the process and the quality of the final product, maintaining uniform composition during the process and controlling/understanding the shrinkage in drying and sintering. Furthermore, understanding the tape delamination and film cracking of multilayers as well as of interface fracture modes in multilayers is also an important topic that needs to be considered and understood.

In the present PhD thesis the focus is on the numerical modelling of the tape casting process of functionally graded ceramic materials for fuel cell applications as well as magnetic refrigeration. Models to simulate the shaping of monolayer/multilayer and graded materials by tape casting are developed. The emphasis is on analyzing the entry flow of multiple slurries from the reservoir into the doctor-blade region as well as the exit region where a free surface (meniscus) forms. This encompasses a detailed fluid model capable of tracking the material flow/deformation taking the formation of the free surface into account. In the work it was chosen to focus on developing analytical/numerical flow solvers in both
Ansys Fluent and Matlab.
Analytical approaches for fluid flow analysis in the tape casting process showed that a relative good agreement could be achieved between the results of the modelling and the experimental data. The study, furthermore, demonstrated that the aforementioned agreement was increased by improving the steady state model with a quasi-steady state analytical model. In order to control the most important process parameter, tape thickness, the two-doctor blade configuration was also modeled analytically. The model was developed to control the tape thickness based on the machine configuration and the material constants. Many of the affecting parameters in the process were embedded and they can easily be varied to evaluate their influence.

This study showed that using computational fluid dynamics (CFD) the process can be modeled with more details in order to better control the produced tapes. Very importantly, the free surface of the ceramic as leaving the doctor blade region was modeled. The rheological behavior of the ceramic slurry was also taken into account. The influence of the main process parameters, i.e. the substrate velocity, the initial slurry load, and the doctor blade height, were investigated.

Numerical models were developed to track the migration of the particles inside the ceramic slurry. The results showed the presence of some areas inside the ceramic in which the concentration of the particles is higher compared to other parts, creating the resulting packing structure. And finally a numerical code was developed to simulate the drying process. The results showed that the mass loss due to the evaporation is increasing close to linearly with the drying time corresponding to an almost constant drying rate. However, the rate starts to decrease after some time in the simulation. This is in good agreement with the real life process where the drying categorized into two stages: (1) constant rate period (CRP), in which the rate of evaporation per unit area of the drying surface is independent of time, (2) falling rate period (FRP), in which the evaporation rate is reduced, as a consequence of low migration of the water from the bottom layers to the top ones due to diffusion (which is highly dependent to the temperature).
Nanosecond laser ablation and deposition of silver, copper, zinc and tin
Nanosecond pulsed laser deposition of different metals (Ag, Cu, Sn, Zn) has been studied in high vacuum at a laser wavelength of 355 nm and pulse length of 6 ns. The deposition rate is roughly similar for Sn, Cu and Ag, which have comparable cohesive energies, and much higher for the deposition of Zn which has a low cohesive energy. The deposition rate for all metals is strongly correlated with the total ablation yield, i.e., the total mass ablated per pulse, reported in the literature except for Sn, for which the deposition rate is low, but the total ablation yield is high. This may be explained by the continuous erosion by nanoparticles during deposition of the Sn films which appear to have a much rougher surface than those of the other metals studied in the present work.

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Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Electrofunctional materials
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Progress in magnetic refrigeration and future challenges

Since a regenerative magnetic cooling cycle was first demonstrated in 1976, many developments have been made in the areas of system modeling, magnetocaloric materials and system design. Systems have gone from laboratory demonstrators using superconducting magnets to near commercial systems using more practical permanent magnets and use multi-material regenerators. Novel magnetocaloric material systems show potentially higher magnetocaloric properties than gadolinium and its alloys while reducing the cost of the raw materials. Detailed numerical models have been developed and show that magnetic refrigerators have the potential for high efficiency. However, reported device COPs for laboratory devices are still well below commercially available vapor compression systems. In order to significantly improve AMR efficiency, several loss mechanisms must be reduced and other aspects of system design, such as the drive system, must be better understood. Here, some major loss mechanisms are presented and modeling tools and design solutions are presented. Other challenges that must be overcome before the technology can become commercially viable are also discussed.

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Pulsed laser deposition of ZnS and Cu2SnS3 multicompartment targets

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Room Temperature Creation of High Mobility Two-Dimensional Electron Gases at Complex Oxide Interfaces

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Center for Electron Nanoscopy
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Room Temperature Epitaxial Growth of Complex Oxide Interfaces with High Mobility Two-Dimensional Electron Gases

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Room temperature formation of high-mobility two-dimensional electron gases at crystalline complex oxide interfaces

Well-controlled sub-unit-cell layer-by-layer epitaxial growth of spinel alumina is achieved at room temperature on a TiO2-terminated SrTiO3 single-crystalline substrate. By tailoring the interface redox reaction, 2D electron gases with mobilities
exceeding 3000 cm¹² V⁻¹ s⁻¹ are achieved at this novel oxide interface.

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  - Scopus rating (2015): CiteScore 18.5
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  - Web of Science (2014): Indexed yes
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  - ISI indexed (2013): ISI indexed yes
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  - Web of Science (2011): Impact factor 1.796
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 2
  - Web of Science (2010): Impact factor 1.804
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 2
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 2
Since 1990s, oxide thermoelectrics have been considered as promising thermoelectric (TE) materials due to their non-toxicity, low-cost, and chemical stability at high temperatures. Studied results show great potential for applications in thermoelectric power generator (TEG) at high temperature and thus have drawn attentions over the years. However, oxides TEGs are still not used broadly due to their low performance. This thesis targets the research and development of using these materials in high temperatures range using high conversion efficiency TEG based modules. This study demonstrates an effective way to improve the efficiency of oxide TEG by segmentation of oxide materials with other high-performance non-oxide materials, thereby, extending the temperature range.

This thesis was started by developing of n-type oxide material e.g. CaMnO₃ as possible alternative n-type candidate for a more stable high temperature material. In this study, thermoelectric properties from 300 to 1200 K of Ca₉₀ₓY₀.₁Mn₁₋ₓFeₓO₃ for 0 ≤ x ≤ 0.25 were systematically investigated in term of Y and Fe co-doping at the Ca- and Mn-sites, respectively. It was found that with increasing the content of Fe doping, the Seebeck coefficient of Ca₉₀ₓY₀.₁Mn₁₋ₓFeₓO₃ tended to increase, while the tendency towards the electrical conductivity was more complicated. Thermal conductivity of the Fe-doped samples showed a lower value than that of the non-doped sample. The maximum dimensionless figure-of-merit, zT was found to be improved about 20% for the sample with x = 0.05 as compared to that of the x = 0 sample at 1150 K. High-performance segmented legs/unicouples based on oxide materials are first designed by numerical modelling. The criteria of material selection for segmentation are based on their "efficiency ratio" described the total conversion efficiency per the materials cost and their compatibility factors. The numerical modeling results (chapter 3) showed that the maximum theoretical conversion efficiency of segmented legs/unicouples could be over 10%, which is more than twice as compared with the one comprised from non-segmented oxide elements. The calculation also takes into account the interfacial contact resistances to evaluate the influence on the total conversion efficiency. The obtained modeling results provide useful tools for designing future low-cost, high-performance segmented TEGs. A high-performance segmented oxide-based module comprising of 4-unicouples using segmentation of the half-Heusler Ti₀.₃Zr₀.₃₅Hf₀.₃₅CoSb₀.₈Sn₀.₂ and the misfit-layered cobaltite Ca₃Co₄O₉₊δ as the p-leg and 2% Al-doped ZnO as the n-leg was successfully fabricated and characterized. The results (presented in Chapter 5) show that at a temperature difference of 700 K, the maximum output power density attains a value of ~6.5 kW/m², which is three times higher than that of a non-segmented oxide module under the same condition. Initial long-term stability test of the module at hot and cold side temperature of 1073/444 K showed a promising result, although a slight degradation tendency could be observed after 48 hours of operating in air. Nevertheless, the total conversion efficiency of this segmented module is still low less than 2%, and needs to be further improved. A degradation mechanism was observed, which attributed to the increase in the interfacial contact resistance between the n-type material (doped ZnO) and the metal electrode. The next study (Chapter 6) focuses on enhancing the efficiency of a single oxide-based segmented leg by further reducing the contact resistance and employing materials with better TE properties, i.e. a p-type leg that consists of misfit-layered cobaltite Ca₂.₈Lu₀.₁₅Ag₀.₀₅Co₄O₉₊δ nano-composite and the half-Heusler Ti₀.₃Zr₀.₃₅Hf₀.₃₅CoSb₀.₈Sn₀.₂ alloy. For the first time, a maximum conversion efficiency as high as ~5% at a ΔT = 756 K was measured. This high efficiency segmented leg is also tested for over two weeks at the hot and cold side temperatures of 1153/397 K, showing good durability as a result of stable, low electrical resistance contacts.
Strain in the mesoscale kinetic Monte Carlo model for sintering

Shrinkage strains measured from microstructural simulations using the mesoscale kinetic Monte Carlo (kMC) model for solid state sintering are discussed. This model represents the microstructure using digitized discrete sites that are either grain or pore sites. The algorithm used to simulate densification by vacancy annihilation removes an isolated pore site at a grain boundary and collapses a column of sites extending from the vacancy to the surface of sintering compact, through the center of mass of the nearest grain. Using this algorithm, the existing published kMC models are shown to produce anisotropic strains for homogeneous powder compacts with aspect ratios different from unity. It is shown that the line direction biases shrinkage strains in proportion the compact dimension aspect ratios. A new algorithm that corrects this bias in strains is proposed; the direction for collapsing the column is determined by choosing a random sample face and subsequently a random point on that face as the end point for an annihilation path with equal probabilities. This algorithm is mathematically and experimentally shown to result in isotropic strains for all samples regardless of their dimensions. Finally, the microstructural evolution is shown to be similar for the new and old annihilation algorithms.

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, Sandia National Laboratories, San Diego State University
Contributors: Bjørk, R., Frandsen, H. L., Tikare, V., Olevsky, E., Pryds, N.
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BFI (2016): BFI-level 1
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Web of Science (2016): Impact factor 2.292
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.3 SJR 0.953 SNIP 1.289
Web of Science (2015): Impact factor 2.086
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.47 SJR 1.098 SNIP 1.612
Web of Science (2014): Impact factor 2.131
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.15 SJR 0.951 SNIP 1.306
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.14 SJR 1.006 SNIP 1.616
Web of Science (2012): Impact factor 1.878
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Structural instability and electrical properties in epitaxial Er$_2$O$_3$-stabilized Bi$_2$O$_3$ thin films

Bismuth oxide based materials exhibit the highest oxygen ion conductivities, making them of great interest for use in energy conversion devices such as solid oxide fuel cells. However, these materials exhibit chemical and thermal instabilities and understanding and their stabilization is an actively pursued research goal. In this study, we investigate the structural and electrical properties of erbium oxide stabilized bismuth oxide (Er$_0.4$Bi$_1.6$O$_3$ – $\delta$) as thin films. These are deposited by pulsed laser deposition onto several single crystal substrates (MgO, Al$_2$O$_3$ and SrTiO$_3$). The films show new forms of instabilities, both upon aging treatments in air and even under conductivity measurements, with remarkable changes in the film composition and microstructure. © 2014 Published by Elsevier B.V.
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BFI (2018): BFI-level 1
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Web of Science (2017): Impact factor 2.751
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Impact factor 2.354
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.5 SJR 0.802 SNIP 1.016
Web of Science (2015): Impact factor 2.38
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.62 SJR 0.837 SNIP 1.282
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BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.35 SJR 0.903 SNIP 1.269
Web of Science (2013): Impact factor 2.112
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.31 SJR 1.051 SNIP 1.253
Web of Science (2012): Impact factor 2.046
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.96 SJR 1.376 SNIP 1.615
Web of Science (2011): Impact factor 2.646
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Impact factor 2.496
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.515 SNIP 1.617
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.292 SNIP 1.384
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.239 SNIP 1.541
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.093 SNIP 1.423
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.18 SNIP 1.55
Web of Science (2004): Indexed yes
The influence of non-magnetocaloric properties on the performance in parallel-plate AMRs

The performance of Active Magnetic Regenerators (AMR) does not depend solely on the magnetocaloric effect of their constituents. Rather, it depends on several additional parameters, including, magnetic field, geometry (hydraulic diameter, cross-sectional area, regenerator length etc.), thermal properties (conductivity, specific heat and mass density) and operating parameters (utilization, frequency, number of transfer units etc.). In this paper we focus on the influence of three parameters on regenerator performance: 1) Solid thermal conductivity, 2) magnetostatic demagnetization and 3) flow maldistribution due to geometrically non-uniform regenerators. It is shown that the AMR performance is optimal at an intermediate value of the solid thermal conductivity for many operating conditions. The magnetostatic demagnetization is shown to have a significant influence on the AMR performance, giving a strong dependence on the orientation of the applied field and the regenerator geometry. Finally, the flow maldistribution of non-uniform regenerator geometries is found to degrade the AMR performance even at minor deviations from perfectly homogeneous regenerator matrices. This paper reflects a summary of various recently published results.

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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.44 SJR 1.349 SNIP 1.532
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.6 SJR 1.619 SNIP 2.086
Towards high efficiency segmented thermoelectric unicouples

Segmentation of thermoelectric (TE) materials is a widely used solution to improve the efficiency of thermoelectric generators over a wide working temperature range. However, the improvement can only be obtained with appropriate material selections. In this work, we provide an overview of the theoretical efficiency of the best performing unicouples designed from segmenting the state-of-the-art TE materials. The efficiencies are evaluated using a 1D numerical model which includes all thermoelectric effects, heat conduction, Joule effects and temperature dependent material properties, but neglects contact resistance and heat losses. The calculations are performed for a fixed cold side temperature of 300K and different hot side temperatures of 700, 900, and 1100 K. We confirm that without taking into account the compatibility of TE materials, segmentation can even decrease the total efficiency. Choosing the TE materials carefully, one is, however, rewarded by a significant improvement in the total efficiency.

General information
**Transport Properties of the γ-Al₂O₃/SrTiO₃ Heterostructure**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Christensen, D. V., Chen, Y., Smith, A., Pryds, N.
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Event: Abstract from 21st International Workshop on Oxide Electronics, Lake George, NY, United States.
Electronic versions:
Transport_Properties.pdf

**Visible-light-enhanced gating effect at the LaAlO₃/SrTiO₃ interface**

Electrostatic gating field and light illumination are two widely used stimuli for semiconductor devices. Via capacitive effect, a gate field modifies the carrier density of the devices, while illumination generates extra carriers by exciting trapped electrons. Here we report an unusual illumination-enhanced gating effect in a two-dimensional electron gas at the LaAlO₃/SrTiO₃ interface, which has been the focus of emergent phenomena exploration. We found that light illumination decreases, rather than increases, the carrier density of the gas when the interface is negatively gated through the SrTiO₃ layer, and the density drop can be 20 times as large as that caused by the conventional capacitive effect. This effect is further found to stem from an illumination-accelerated interface polarization, an originally extremely slow process. This unusual effect provides a promising controlling of the correlated oxide electronics in which a much larger gating capacity is demanding due to their intrinsic larger carrier density.

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Scopus rating (2015): CiteScore 11.23 SJR 6.287 SNIP 2.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 10.77 SJR 6.41 SNIP 3.034
Web of Science (2014): Impact factor 11.47
A high-mobility two-dimensional electron gas at the spinel/perovskite interface of \( \gamma \)-Al\(_2\)O\(_3\)/SrTiO\(_3\).

The discovery of two-dimensional electron gases at the heterointerface between two insulating perovskite-type oxides, such as LaAlO\(_3\) and SrTiO\(_3\), provides opportunities for a new generation of all-oxide electronic devices. Key challenges remain for achieving interfacial electron mobilities much beyond the current value of approximately 1,000 cm\(^2\)V\(^{-1}\)s\(^{-1}\) (at low temperatures). Here we create a new type of two-dimensional electron gas at the heterointerface between SrTiO\(_3\) and a spinel \( \gamma \)-Al\(_2\)O\(_3\) epitaxial film with compatible oxygen ions sublattices. Electron mobilities more than one order of magnitude higher than those of hitherto-investigated perovskite-type interfaces are obtained. The spinel/perovskite twodimensional electron gas, where the two-dimensional conduction character is revealed by quantum magnetoresistance oscillations, is found to result from interface-stabilized oxygen vacancies confined within a layer of 0.9 nm in proximity to the interface. Our findings pave the way for studies of mesoscopic physics with complex oxides and design of high-mobility all-oxide electronic devices.
A high-mobility two-dimensional electron gas at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃

The realization of high-mobility 2DEGs in epitaxially grown heterostructures made of traditional semiconductors is at the heart of present electronics, which has led to a wealth of new physical phenomena as well as new electronic and photonic devices over the past few decades. 2DEGs at the interface between insulating complex oxides not only provide a wealth of opportunities to study mesoscopic physics with strongly correlated electrons confined in nanostructures, but also show promise for multifunctional all-oxide devices with probably even richer behavior than those we experienced in semiconductor devices.

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State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, Imaging and Structural Analysis
Contributors: Chen, Y., Trier, F., Christensen, D. V., Andersen, N. H., Kasama, T., Zhang, W., Linderoth, S., Pryds, N.
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A high-mobility two-dimensional electron gas at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃ grown by pulsed laser deposition

General information
A Two-Dimensional Electron Gas at the Spinel/Perovskite Interface of γ-Al₂O₃/SrTiO₃ with Carrier Mobility Exceeding 100,000 cm²V⁻¹s⁻¹

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, Imaging and Structural Analysis, Chinese Academy of Sciences, Leibniz Institute for Solid State and Materials Research Dresden (IFW), University of Copenhagen
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Camber Evolution and Stress Development of Porous Ceramic Bilayers During Co-Firing
Camber evolution and stress development during co-firing of asymmetric bilayer laminates, consisting of porous Ce₀.₉Gd₀.₁O₁.₉₅ gadolinium-doped cerium oxide (CGO) and La₀.₈₅Sr₀.₁₅MnO₃ lanthanum strontium manganate (LSM)-CGO were investigated. Individual layer shrinkage was measured by optical dilatometer, and the uniaxial viscosities were determined as a function of layer density using a vertical sintering approach. The camber evolution in the bilayer laminates was recorded in situ during co-firing and it was found to correspond well with the one predicted by the theoretical model. The estimated sintering mismatch stress in co-fired CGO-LSM/CGO bilayer laminates was significantly lower than general sintering stresses expected for free sintering conditions. As a result, no co-firing defects were observed in the bilayer laminates, illustrating an acceptable sintering compatibility of the ceramic layers.

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Controlling interfacial states in amorphous/crystalline LaAlO$_3$/SrTiO$_3$ heterostructures by electric fields

The tunable metal-insulator transition in crystalline LaAlO$_3$/SrTiO$_3$ heterostructures constitutes a central element in the range of remarkable interface properties that has made this oxide system subject to extensive research. Recently, metallic interfaces have also been realized when depositing amorphous LaAlO$_3$ films on SrTiO$_3$. Here, we present a non-volatile and reversible tuning of the interface conductivity by more than 3 orders of magnitude at room temperature by applying an electric field to such amorphous/crystalline heterostructures with amorphous LaAlO$_3$ film thicknesses of 2 nm. We show that the tunability is strongly temperature dependent, and demonstrate a simple protocol for enhancing the tunability. © 2013 American Institute of Physics.
Controlling the conductivity of amorphous LaAlO3/SrTiO3 interfaces by in-situ application of an electric field during fabrication

Amorphous-LaAlO3/SrTiO3 interfaces present metallic conductivity similar to those found in their all-crystalline counterparts. Here, the conductivity of amorphous-LaAlO3/SrTiO3 interfaces is modified by an external electric field applied in-situ with a biased truncated cone electrode (−10V ≤ Vbias ≤ 20V) during film growth. By modulating the charge balance of the arriving plasma species, interfacial conduction of the amorphous-LaAlO3/SrTiO3 heterostructures shifts from metallic to insulating via a semiconducting-like characteristic transport mode. This remarkable behavior is explained by a modification of the Al-ion flux impinging the SrTiO3 surface, which alters the amount of near-interface oxygen vacancies being formed at the SrTiO3 surface.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Naples Federico II
Degradation of the interfacial conductivity in LaAlO₃/SrTiO₃ heterostructures during storage at controlled environments

The remarkable discovery of a two-dimensional electron gas confined at the interface of the two oxide band-insulators SrTiO₃ (STO) and LaAlO₃ (LAO) has spurred a great interest in the heterostructure leading to the discovery of a plethora of other exciting properties. Recently, the formation of the interfacial electron gas has also been shown possible when LAO is deposited on STO at room temperature, which leads to the growth of amorphous LAO (a-LAO). Here, we study the development of the interfacial conductivity of LAO/STO heterostructures with crystalline and amorphous LAO top layers in different controlled environments over time. The interfacial conductivity is found to degrade with a strong dependence on the thickness, the crystallinity of the deposited layer and the storage environment. A mechanism for the degradation is proposed and is further utilized to significantly reduce the rate of degradation.

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Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
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Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
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Development of Thermoelectric Power Generators for high temperature Waste Heat Recovery

By converting heat directly into electricity, thermoelectric generators (TEGs) provide a very promising solution for emerging energy saving and environmental issues. These devices could be incorporated in a variety of applications, in particular those making use of waste heat recovery. To expand the range of application of TEGs, new more efficient thermoelectric materials and devices are needed. In this report, the development progress for high temperature TEGs using thermoelectric materials developed at DTU Energy Conversion and Storage is presented and the recent achievements on non-segmented and segmented oxides-based TEGs are highlighted and compared with the results reported so far on literatures. By combining a thermoelectric oxide and half-Heusler alloy, a novel segmented TEG obtained a maximum output power, which is 7 times better than that of a non-segmented TEG using pure oxides. Various issues related to the fabrication of TEGs and long-term stability test will be briefly discussed.

Effects of Synthesis and Spark Plasma Sintering Conditions on the Thermoelectric Properties of Ca$_3$Co$_4$O$_{9+\delta}$

Ca$_3$Co$_4$O$_{9+\delta}$ samples were synthesized by solid-state (SS) and sol-gel (SG) reactions, followed by spark plasma sintering under different processing conditions. The synthesis process was optimized and the resulting materials characterized with respect to their microstructure, bulk density, and thermoelectric transport properties. High power factors of about 400 μW/m·K$^2$ and 465 μW/m·K$^2$ (at 800°C) were measured for SS and SG samples, respectively. The improved thermoelectric performance of the SG sample is believed to originate from the smaller particle sizes and better grain alignment. The SG method is suggested to be a beneficial means of obtaining high-performance thermoelectric materials of Ca$_3$Co$_4$O$_{9+\delta}$ type.
Fabrication and performance of high temperature segmented thermoelectric oxide-based module

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Le, T. H., Pham, H. N., Han, L., Holgate, T., Van Nong, N., Linderoth, S., Pryds, N.
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Event: Abstract from 32nd International Conference on Thermoelectrics, Kobe, Japan.
High-mobility two-dimensional electron gases at oxide interfaces: Origins and opportunities.
Our recent experimental work on metallic and insulating interfaces controlled by interfacial redox reactions in SrTiO3-based heterostructures is reviewed along with a more general background of two-dimensional electron gas (2DEG) at oxide interfaces. Due to the presence of oxygen vacancies at the SrTiO3 surface, metallic conduction can be created at room temperature in perovskite-type interfaces when the overlayer oxide ABO3 has Al, Ti, Zr, or Hf elements at the B sites. Furthermore, relying on interface-stabilized oxygen vacancies, we have created a new type of 2DEG at the heterointerface between SrTiO3 and a spinel g-Al2O3 epitaxial film with compatible oxygen ion sublattices. This 2DEG exhibits an electron mobility exceeding 100000 cm²·V⁻¹·s⁻¹, more than one order of magnitude higher than that of hitherto investigated perovskite-type interfaces. Our findings pave a way for the design of high-mobility all-oxide electronic devices and open a route toward the studies of mesoscopic physics with complex oxides.

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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.8 SJR 0.263 SNIP 0.406
Web of Science (2017): Impact factor 1.321
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.57 SJR 0.339 SNIP 0.526
Web of Science (2016): Impact factor 1.223
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.59 SJR 0.411 SNIP 0.678
Web of Science (2015): Impact factor 1.436
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.74 SJR 0.495 SNIP 0.872
Web of Science (2014): Impact factor 1.603
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.52 SJR 0.399 SNIP 0.781
Web of Science (2013): Impact factor 1.392
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.6 SJR 0.312 SNIP 0.577
Web of Science (2012): Impact factor 1.148
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
High-temperature Thermoelectric Properties of Ca$_{0.9}$Y$_{0.1}$Mn$_{1-x}$Fe$_x$O$_3$ ($0 \leq x \leq 0.25$)

Polycrystalline compounds of Ca$_{0.9}$Y$_{0.1}$Mn$_{1-x}$Fe$_x$O$_3$ for $0 \leq x \leq 0.25$ were prepared by solid-state reaction, followed by spark plasma sintering process, and their thermoelectric properties from 300 to 1200 K were systematically investigated in terms of Y and Fe co-doping at the Ca- and Mn-sites, respectively. Crystal structure refinement revealed that all the investigated samples have the O'-type orthorhombic structure, and the lattice parameters slightly increased with increasing Fe concentration, causing a crystal distortion. It was found that with increasing the content of Fe doping, the Seebeck coefficient of Ca$_{0.9}$Y$_{0.1}$Mn$_{12}$xFe$_x$O$_3$ tended to increase, while the tendency toward the electrical conductivity was more complicated. The highest power factor was found to be $2.1 \times 10^{-4}$ $\text{W/mK}^2$ at 1150 K for the sample with $x = 0.05$ after annealing at 1523 K for 24 h in air. Thermal conductivity of the Fe-doped samples showed a lower value than that of the $x = 0$ sample, and the highest dimensionless figure of merit, ZT was found to be improved about 20 % for the sample with $x = 0.05$ as compared to that of the $x = 0$ sample at 1150 K.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Functional organic materials, Management, Hanoi University of Science and Technology, Aarhus University
Pages: 2817-2822
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.83 SJR 0.807 SNIP 1.064
Web of Science (2017): Impact factor 2.993
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.769 SNIP 1.072
Web of Science (2016): Impact factor 2.599
High Temperature Thermoelectric Properties of Y and Fe codopants in Ca$_3$Co$_4$O$_9+\delta$

A series of Ca$_{3-x}$Y$_x$Co$_{4-y}$Fe$_y$O$_9+\delta$ powders was synthesized by auto-combustion reaction and densified with spark plasma sintering (SPS) processing. The electrical resistivity and the Seebeck coefficient increase with the increasing yttrium content, while the electrical resistivity decreases with the iron content below 0.05. The reasons for the increase in both the electrical resistivity and the Seebeck coefficient with the yttrium substitution are due to the carrier (Co$^{4+}$) number reduction in CdI$_2$ type CoO$_2$ layer. In contrary, iron substitution below certain content may only occur in rocksalt type Ca$_2$CoO$_3$ layer resulting in the increase of the carrier number. The Y and Fe co-dopants effect on the thermal conductivity is not significant even though the yttrium heavier atomic weight is expected as an effective phonon scattering site. At 800 °C, the improved power factor of 520 μW/m•K$^2$ from x=0.2 and y=0.03 sample was obtained, compared with the power factor of 450 μW/m•K$^2$ from pure Ca$_3$Co$_4$O$_9+\delta$, which demonstrates the improvement of Ca$_3$Co$_4$O$_9+\delta$ thermoelectric properties with co-dopants yttrium and iron.

Influence of porosity on densification and grain growth kinetics of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ tape

Gadolinium doped-ceria (CGO) is an important material that offers high stability, tolerance against harsh environments and high ionic and electronic conductivity at high temperatures. For most of its applications, CGO is applied as a thin dense layer on a porous support structure. However, highly porous layer allowing gas flow is necessary in catalytic and in gas purification devices. During the sintering with shrinkage, the total solid volume is maintained to be a constant value but the shape and size of each particle change with the formation of grain boundaries. This change in solid particles is accompanied by the change of shape, size and fraction of pores in a given volume. Therefore, porosity can be treated as an extra phase during sintering study. In this work, we presented the densification and grain growth behaviour of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ tape cast layers with different percentage of porosity. The emphasis was put on the effect of porosity on densification and grain growth kinetics. Derived from the sintering constitutive laws, the densification and grain growth kinetics were experimentally characterized and analyzed. Furthermore, the activation energies for viscous flow were determined from master viscosity curves, which are comparable to the kinetic values obtained from densification and grain growth. It is indicated that porosity has negligible effect on densification kinetics, but high porosity decreases the chance of particle contact, and grain boundary mobility is therefore slowed, which leads to slower grain growth.

Laser deposition rates of thin films of selected metals and alloys

Thin films of Cu, Zn and Sn as well as mixtures of these elements have been produced by Pulsed Laser Deposition (PLD). The deposition rate of single and multicomponent metallic targets was determined. The strength of PLD is that the stoichiometry of complex compounds, even of complicated alloys or metal oxides, can be preserved from target to film. We apply this technique to design films of a mixture of Cu, Zn and Sn, which are constituents of the chalcogenide CZTS, which has a composition close to Cu$_2$ZnSnS$_4$. This compound is expected to be an important candidate for absorbers in new solar cells.

The experiments have been carried out at a laser wavelength of 355 nm in vacuum with a PLD chamber at DTU Fotonik,
Risø Campus. The deposition rates have been measured by a quartz crystal microbalance. At a laser fluence of 2 J/cm² the total ablated yield of copper is about 1x10¹⁵ atoms per pulse. The film deposition rate is typically 100 times lower because not all the ablated atoms do arrive at the substrate. The deposition rate of copper is about 1x10¹³ atoms/cm² per pulse in a direction normal to the target surface, which is 6 times lower than that of Sn and 4 times lower than that of Zn. Results for alloys of the different elements as well as compounds with S will be presented.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Cazzaniga, A. C., Canulescu, S., Schou, J., Pryds, N.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from 12th International Conference on Laser Ablation (COLA 2013), Ischia, Italy.
Electronic versions:
prod21383214158512.Schou_02.pdf
Source: dtu
Source-ID: u::9253
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2013

Modeling Kinetics of Distortion in Porous Bi-layered Structures
Shape distortions during constrained sintering experiment of bi-layer porous and dense cerium gadolinium oxide (CGO) structures have been modeled. Technologies like solid oxide fuel cells require co-firing thin layers with different green densities, which often exhibit differential shrinkage because of different sintering rates of the materials resulting in undesired distortions of the component. An analytical model based on the continuum theory of sintering has been developed to describe the kinetics of densification and distortion in the sintering processes. A new approach is used to extract the material parameters controlling shape distortion through optimizing the model to experimental data of free shrinkage strains. The significant influence of weight of the sample (gravity) on the kinetics of distortion is taken in to consideration. The modeling predictions indicate good agreement with the results of sintering of a bi-layered CGO system in terms of evolutions of bow, porosities and also layer thickness.

General information
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Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Ceramic Engineering & Science, San Diego State University
Contributors: Tadesse Molla, T., Frandsen, H. L., Bjørk, R., Ni, D. W., Olevsky, E., Pryds, N.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Impact factor 3.794
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Impact factor 3.454
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.03 SJR 1.135 SNIP 1.817
Web of Science (2015): Impact factor 2.933
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Modeling sintering of multilayers under influence of gravity

There is a tendency for multiple functional ceramic layers used in various applications to have increasing surface areas and decreasing thicknesses. Sintering samples with such geometry is challenging, as differential shrinkage of the layers causes undesired distortions. In this work, a model, which describes the combined effect of sintering and gravity of thin multilayers, is derived and later compared with experimental results. It allows for consideration of both uniaxial and biaxial stress states. The model is based on the Skorohod-Olevsky viscous sintering framework, the classical laminate theory and...
the elastic-viscoelastic correspondence principle. The modeling approach is then applied to illustrate the effect of gravity during sintering of thin layers of cerium gadolinium oxide (CGO), and it is found to be significant. © 2012 The American Ceramic Society.
Nanostructured oxide materials and modules for high temperature power generation from waste heat

A large amount of thermal energy that emitted from many industrial processes is available as waste heat. Thermoelectric power generators that convert heat directly into electricity can offer a very promising way for waste heat recovery. However, the requirements for this task place in the materials are not easily satisfied by conventional thermoelectric materials. Not only they must possess a sufficient thermoelectric performance, they should also be stable at high temperatures, nontoxic and low-cost comprising elements, and must be also able to be processed and shaped cheaply. Oxides are among the strongest candidate materials for this purpose. In this review, the progress in the development of two representative p- and n-type novel oxide materials based on Ca$_{3}$Co$_{4}$O$_{9}$ and doped-ZnO is presented. Thermoelectric modules built up from these oxides were fabricated, tested at high temperatures, and compared with other similar oxide modules reported in the literature. A maximum power density of 4.5 kW/m$^2$ was obtained for an oxide module comprising of 8 p-n couples at a temperature difference of 496 K, an encouraging result in the context of the present high temperature oxide modules.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Van Nong, N., Pryds, N.
Number of pages: 8
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Publication information

Journal: Advances in Natural Sciences: Nanoscience and Nanotechnology
Volume: 4
ISSN (Print): 2043-6254
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.7 SJR 0.442 SNIP 0.625
Web of Science (2017): Indexed yes
Performance analysis of a rotary active magnetic refrigerator

Performance results for a novel rotary active magnetic regenerator (AMR) and detailed numerical model of it are presented. The experimental device consists of 24 regenerators packed with gadolinium (Gd) spheres rotating inside a four-pole permanent magnet with magnetic field of 1.24T. A parametric study of the temperature span, cooling power, coefficient of performance (COP) and efficiency of the system was carried out over a range of different hot reservoir temperatures, volumetric flow rates and cooling powers. Detailed modeling of the AMR using a 1D model was performed and compared with the experimental results. An overall mapping of the thermal losses of the system was performed, and good agreement between the experimental and numerical results was found when parasitic heat losses were subtracted from the modeling results. The performance of the system was evaluated via the COP, the exergetic-equivalent cooling power (ExQ), and the overall second law efficiency, \( \eta_{2nd} \). Losses mapping indicated that friction and thermal leakage to the ambient are the most important contributors to the reduction of the system performance. Based on modeling results, improvements on the flow distributor design and reduction of the cold end thermal parasitic losses are expected to enhance the efficiency of the system. For an operating frequency of 1.5Hz, a volumetric flow rate of 400L/h, a hot reservoir temperature of 297.7K, and thermal loads of 200 and 400W, the obtained temperature spans, \( \delta T_S \), were 16.8K and 7.1K, which correspond to COPs of 0.69 and 1.51, respectively. The maximum overall second-law efficiency was 5.6% for a \( \delta T_S \) of 12.9K at 500L/h and 400W. © 2013 Elsevier Ltd.
Preparation and characterization of segmented p-type Ti$_{0.3}$Zr$_{0.35}$Hf$_{0.35}$CoSb$_{0.8}$Sn$_{0.2}$/Ca$_3$Co$_4$O$_{9+\delta}$

Misfit-layered cobaltite Ca$_3$Co$_4$O$_{9+\delta}$ is considered as good p-type thermoelectric material in high temperature region (950 - 1100 K), while half-Heusler (HH) Ti$_{0.32}$Zr$_{0.35}$Hf$_{0.35}$CoSb$_{0.8}$Sn$_{0.2}$ is high performance p-type material at temperatures below 950 K. In this work, oxide Ca$_3$Co$_4$O$_{9+\delta}$ is segmented with HH using an electrically conductive adhesive and brazing joining technique. The thermoelectric properties of the component materials as well as the interfacial resistance at high temperatures were characterized as a function of temperature up to 1100 K, and the results are discussed in details.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Johannes Gutenberg University
Contributors: Le, T. H., Han, L., Stamate, E., Pham, H. N., Balke, B., Linderoth, S., Van Nong, N., Pryds, N.
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from 2013 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Source: dtu
Source-ID: u::9746
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Sintering of bi-layered porous structures: Stress development and shape evolution

Ce$_{0.95}$Gd$_{0.05}$O$_{1.95}$ (CGO) and (La, Sr)MnO$_3$ (LSM) are electro-ceramics materials with high potential for several electrochemical applications such as solid Oxide Fuel Cell (SOFC), gas separation membranes, and flue gas purification application. In this work, porous CGO and LSM/CGO single layers were prepared by tape casting, and CGO-LSM/CGO bi-layer structures were obtained by lamination. The shrinkage characteristics of individual layers were measured by optical dilatometry and the uniaxial viscosity of layers was determined as a function of temperature and density using a vertical sintering approach. The distortion in the bi-layer configurations was experimentally recorded and compared with the analytical calculations. The sintering mismatch stress was calculated from both the camber development and linear strain rate mismatch, which showed a good agreement.

General information
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Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Electrofunctional materials
Contributors: Ni, D. W., Esposito, V., Ramousse, S., Pryds, N.
Publication date: 2013
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Event: Abstract from 8th International Conference on High-Performance Ceramics, Chongqing, China.
Source: dtu
Source-ID: u::9467
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Sintering of Multilayered Porous Structures: Part I-Constitutive Models

Theoretical analyses of shrinkage and distortion kinetics during sintering of bilayered porous structures are carried out. The developed modeling framework is based on the continuum theory of sintering; it enables the direct assessment of the cofiring process outcomes and of the impact of process controlling parameters. The derived “master sintering curve”-type solutions are capable of describing and optimizing the generic sintering shrinkage and distortion kinetics for various material systems. The approach utilizes the material-specific parameters, which define the relative kinetics of layer shrinkages as the relative intensity of sintering, and employs the conversion between real and specific times of sintering. A novel methodology is also developed for the determination of the ratio of the shear viscosities of the layer’s fully dense materials. This new technique enables the determination of all input parameters necessary for modeling sintering of bilayers using experimental techniques similar to optical dilatometry applied to each individual layer and to a symmetric trilayered porous structure based on the two-layer materials utilized in the bilayered system. Examples of sintering different porous bilayered structures are presented to justify the capability of the model in predicting and optimizing sintering kinetics.

General information
State: Published
Sintering of Multilayered Porous Structures: Part II – Experiments and Model Applications

Experimental analyses of shrinkage and distortion kinetics during sintering of bilayered porous and dense gadolinium-doped ceria Ce0.9Gd0.1O1.95d structures are carried out, and compared with the theoretical models developed in Part I of this work. A novel approach is developed for the determination of the shear viscosities ratio of the layer fully dense materials. This original technique enables the derivation of all the input parameters for the bilayer sintering modeling from one set of optical dilatometry measurements, including the conversion between real and specific times of sintering, the layers’ relative sintering intensity, and the shear viscosities ratio of the layer fully dense materials. These optical dilatometry measurements are conducted simultaneously for each individual layer and for a symmetric trilayered porous structure based on the two layers utilized in the bilayered system. The obtained modeling predictions indicate satisfactory agreement with the results of sintering of a bilayered cerium–gadolinium oxide system in terms of distortion and shrinkage kinetics.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Electrofunctional materials, San Diego State University, Moscow Engineering Physics Institute
Contributors: Ni, D. W., Olevsky, E., Esposito, V., Tadesse Molla, T., Foghmoes, S. P. V., Bjørk, R., Frandsen, H. L., Aleksandrova, E., Pryds, N.
Pages: 2666–2673
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Peer-reviewed: Yes

Publication information
Journal: Journal of the American Ceramic Society
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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 3.06 SJR 0.95 SNIP 1.325
Web of Science (2017): Impact factor 2.956
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1.028 SNIP 1.428
Web of Science (2016): Impact factor 2.841
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.71 SJR 0.995 SNIP 1.37
The effect of particle size distributions on the microstructural evolution during sintering

Microstructural evolution and sintering behavior of powder compacts composed of spherical particles with different particle size distributions (PSDs) were simulated using a kinetic Monte Carlo model of solid state sintering. Compacts of monosized particles, normal PSDs with fixed mean particle radii and a range of standard deviations, and log-normal PSDs with fixed mode and a range of skewness values were studied. Densification rate and final relative density were found to be inversely proportional to initial PSD width. Grain growth was faster during the early stages of sintering for broad PSDs, but the final grain sizes were smaller. These behaviors are explained by the smallest grains in the broader PSDs being consumed very quickly by larger neighboring grains. The elimination of the small grains reduces both the total number of necks and the neck area between particles, which in turn reduces the regions where vacancies can be annihilated, leading to slower densification rates. The loss of neck area causes grain growth by surface diffusion to become the dominant microstructural evolution mechanism, leading to poor densification. Finally, pore size was shown to increase with the width of PSDs, which also contributes to the lower densification rates.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, Sandia National Laboratories
Contributors: Bjørk, R., Tikare, V., Frandsen, H. L., Pryds, N.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 3.06 SJR 0.95 SNIP 1.325
Web of Science (2017): Impact factor 2.956
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1.028 SNIP 1.428
Web of Science (2016): Impact factor 2.841
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.71 SJR 0.995 SNIP 1.37
Web of Science (2015): Impact factor 2.787
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.78 SJR 1.167 SNIP 1.595
Web of Science (2014): Impact factor 2.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.52 SJR 1.16 SNIP 1.48
Web of Science (2013): Impact factor 2.428
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.39 SJR 1.271 SNIP 1.5
Web of Science (2012): Impact factor 2.107
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.45 SJR 0.958 SNIP 1.447
The Influence of Spark Plasma Sintering Temperature on the Microstructure and Thermoelectric Properties of Al,Ga Dual-Doped ZnO

ZnO dual-doped with Al and Ga was prepared by spark plasma sintering using different sintering temperatures. The microstructural evolution and thermoelectric properties of the samples were investigated in detail. The samples obtained with sintering temperature above 1223 K had higher relative densities and higher electronic conductivity than the sample sintered at 1073 K. These results were supported by the solid-state reaction completion rate, which suggested that sintering temperature above 1223 K would be preferable for complete solid-state reaction of the samples. The sintering mechanism of ZnO particles and microstructure evolution at different sintering temperatures were investigated by simulation of the self-Joule-heating effect of the individual particles.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Management
Contributors: Han, L., Le, T. H., Van Nong, N., Pryds, N., Linderoth, S.
Pages: 1573-1581
The influence of α- and γ-Al2O3 Phases on the Thermoelectric Properties of Al-doped ZnO

A systematic investigation of the microstructure and thermoelectric properties of Al-doped ZnO using α- and γ-Al2O3 as dopants was conducted in order to understand the doping effect and its mechanism. The samples were prepared by the spark plasma sintering technique from precursors calcined at various temperatures. Clear differences in microstructure and thermoelectric properties were observed between the samples doped with α- and γ-Al2O3. At any given calcination temperature, γ-Al2O3 resulted in the formation of a larger amount of the ZnAl2O4 phase in the Al-doped ZnO samples. The average grain size was found to be smaller for the γ-Al2O3-doped samples than that for the α-Al2O3-doped ones under the same sintering condition. It is proposed that the ZnAl2O4 phase is the reason for the observed suppression of grain growth and also for the slightly reduced lattice thermal conductivity exhibited by these samples. The γ-Al2O3 promoted the substitution for donor impurities in ZnO, thus resulting in shrinkage of the unit cell volume and an increase in the electrical conductivity compared with the α-Al2O3-doped ZnO. At a calcination temperature of 1173K, the γ-Al2O3-doped sample showed a ZT value of 0.17 at 1173K, which is 27% higher than that of the α-Al2O3-doped sample.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Management, Kyushu University
Contributors: Han, L., Van Nong, N., Le, T. H., Holgate, T., Pryds, N., Ohtaki, M., Linderoth, S.
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Volume: 555
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
Web of Science (2015): Impact factor 3.014
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.13 SJR 1.117 SNIP 1.632
Web of Science (2014): Impact factor 2.999
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.73 SJR 1.059 SNIP 1.583
Thermoelectric Properties of Ca$_3$Co$_4$O$_{9+δ}$ synthesis by Auto-combustion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Wu, N., Holgate, T., Van Nong, N., Pryds, N., Linderoth, S.
Number of pages: 1
Pages: 24
Publication date: 2013

Web of Science (2013): Impact factor 2.726
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.43 SJR 1.246 SNIP 1.57
Web of Science (2012): Impact factor 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.41 SJR 1.164 SNIP 1.463
Web of Science (2011): Impact factor 2.289
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
Web of Science (2010): Impact factor 2.138
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.956 SNIP 1.372
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
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
Scopus rating (2005): SJR 1.088 SNIP 1.208
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.922 SNIP 1.354
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.949 SNIP 1.051
Scopus rating (2002): SJR 0.733 SNIP 1.063
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.634 SNIP 0.966
Scopus rating (2000): SJR 0.707 SNIP 0.938
Scopus rating (1999): SJR 0.744 SNIP 0.927
Original language: English
Keywords: Thermoelectric oxide, Al-doped ZnO, α- and γ-Al2O3, ZnAl2O4, Formation kinetics
Electronic versions:
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DOIs:
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Thermoelectric Properties of Ca$_3$Co$_4$O$_{9+δ}$ synthesis by Auto-combustion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Wu, N., Holgate, T., Van Nong, N., Pryds, N., Linderoth, S.
Number of pages: 1
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Publication date: 2013
Two-dimensional electron gases at a spinel/perovskite complex oxide heterointerface with electron mobilities exceeding 100,000 cm\(^2\) V\(^{-1}\) s\(^{-1}\)

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Chen, Y., Trier, F., Christensen, D. V., Linderoth, S., Pryds, N.
Number of pages: 1
Pages: 77
Publication date: 2013

Two-dimensional electron gases in SrTiO\(_3\)-based complex oxide heterostructures with electron mobilities exceeding 100,000 cm\(^2\) V\(^{-1}\) s\(^{-1}\)

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Chen, Y., Pryds, N.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from EMN West meeting, Energy materials Nanotechnology, Houston, TX, United States.

Utilizing Materials With Controllable Curie Temperatures for Magnetic Actuation Purposes

The magnetic force between a permanent magnet and different blocks of ferromagnetic materials was measured and calculated as a function of distance and temperature in the vicinity of the Curie temperature of the materials. The calculations were carried out using a 3-D finite-element model of the system. On the basis of forces predicted by the model a number of equilibrium points were calculated for a system where the magnetic force on a ferromagnetic block of material is balanced by a linear spring force. It is shown how these calculation procedures can be used as a tool for designing autonomous temperature dependent and temperature adjustable actuation systems. A shunt valve utilizing such a system was designed, built and tested.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Pages: 1159-1162
Publication date: 2013
Peer-reviewed: Yes
Analysis of the sintering stresses and shape distortion produced in co-firing of CGO-LSM/CGO bi-layer porous structures

Gadolinium-doped cerium oxide (CGO) and lanthanum strontium manganate (LSM) are electro-ceramics materials with high potential for several electrochemical applications such as solid Oxide Fuel Cell (SOFC), gas separation membranes, and flue gas purification devices. Especially for novel electrochemical flue gas purification devices, multilayer structures with alternating porous layers of CGO and a LSM/CGO mixture are used to achieve specific functional requirements. In a manufacturing process of such ceramic multilayer devices, co-firing is one of the critical steps as many defects such as cracks, de-lamination and shape distortion can result as a consequence of sintering mismatch stresses caused by the strain rate difference between layers. This work seeks to understand the underlying mechanisms that occur during the co-firing of porous CGO-LSM/CGO bi-layer laminates, by evaluating the sintering mismatch stress and distortion development through modeling and experiments.

A novel magnetic valve using room temperature magnetocaloric materials

Magnetocaloric materials with near-room-temperature tuneable Curie temperatures have been utilized to develop a novel magnetic valve technology. The temperature dependent attractive force between the materials and a permanent magnet assembly is used to actuate valves as a response to temperature changes. This is made possible by the strong temperature dependence of the magnetization close to the Curie temperature of the magnetocaloric materials. Different compositions of both La0.67(Ca,Sr)0.33MnO3 and La(Fe,Co,Si)13 have been considered for use in prototype valves. Based on measured magnetization data a 3D finite element model has been set up to calculate the magnetic force between (graded) blocks of these materials and a permanent magnet assembly. The results have been used to calculate equilibrium points for actuation systems where the magnetic force is balanced by a spring force. On the basis of these calculations two temperature adjustable valve prototypes have been designed, built and tested. Possible applications of near-room-temperature valve actuation based on these materials originally developed for magnetic refrigeration are discussed on the background of the present investigation.
Atomically engineered oxide heterointerfaces: new opportunities for nanionics and nanoelectronics

General information
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Contributors: Chen, Y., Pryds, N.
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Source: dtu
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Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2012

Broadening of the magnetic entropy change in La0.75Ca0.15Sr0.10MnO3
A broad table-like entropy change (ΔS) at room temperature has been observed in the ferromagnetic compound La0.75Ca0.15Sr0.10MnO3, which is analyzed in the concept of Landau theory and with critical exponent analysis obtained from the magnetization measurements. The change in entropy in La0.75Ca0.15Sr0.10MnO3 is discussed in the light of magnetoelastic coupling between the magnetization and the lattice distortion. Application aspects of this unusual broad magnetocaloric effect with relative cooling power of 107 J kg⁻¹ in an applied magnetic field of 1.6 T with an operating temperature range of 93 K around the room temperature are also discussed.

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Scopus rating (2017): CiteScore 2.18 SJR 0.615 SNIP 0.833
Web of Science (2017): Impact factor 2.21
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.14 SJR 0.651 SNIP 0.918
Web of Science (2016): Impact factor 2.084
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.32 SJR 0.692 SNIP 0.989
Web of Science (2015): Impact factor 2.101
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.59 SJR 0.847 SNIP 1.281
Development and Experimental Results from a 1 kW Prototype AMR

A novel rotary magnetic refrigeration device has been designed and constructed following the concepts recently outlined in Bahl et al. (2011). The magnet and flow system design allow for almost continuous usage of both the magnetic field and the magnetocaloric material in 24 cassettes, each containing an active magnetic regenerator (AMR) bed. As outlined in Pryds et al. (2009) a small scale AMR test device has been used for materials choice and optimising operation, with each component being thoroughly characterised and tested before implementation. The prototype design facilitates easy exchange of the 24 cassettes, allowing the testing of different material amounts and compositions. Operating with 2.8 kg of commercial grade Gd spheres a maximum no-span cooling power of 1010 W and a maximum zero load temperature span of 25.4 K have been achieved. For the purpose of actual operation, simultaneous high span and high performance is required. At a heat load of 200 W a high temperature span of 18.9 K has been obtained, dropping to a span of 13.8 K at the higher heat load value of 400 W.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Effects of Synthesis and Processing on the Thermoelectric Properties of Ca₃Co₄O₉₊δ

In the present study, Ca₃Co₄O₉₊δ was synthesized by solid-state and sol-gel reactions followed by spark plasma sintering (SPS) under different conditions such as sintering temperatures, applied pressures and ramping rates. The materials were then characterized with respect to their microstructure, phase purity and thermoelectric properties. With the identical optimal SPS process, the power factor of about 400 µW/m•K² and 465 µW/m•K² (at 800 °C) is measured from samples produced by solid-state and sol-gel reactions respectively, both of these values are higher than the value reported so far. The thermoelectric performance improvement observed for the solid-state and sol-gel reactions suggests that the particle sizes may be a predominant key parameter of the Ca₃Co₄O₉₊δ thermoelectric properties. Smaller particle size (500 nm) as produced in this study by sol-gel synthesis method with optimal SPS process conditions would be a better way to fabricate high performance thermoelectric material Ca₃Co₄O₉₊δ.

E-MRS symposium R: "Laser materials processing for micro and nano applications"
Experimental and numerical results of a high frequency rotating active magnetic refrigerator

Experimental results for a recently developed prototype magnetic refrigeration device at The Technical University of Denmark (DTU) were obtained and compared with numerical simulation results. A continuously rotating active magnetic regenerator (AMR) using 2.8 kg packed sphere regenerators of commercial grade gadolinium (Gd) was employed. With operating frequencies up to 10 Hz and volumetric flow rates up to 600 L/h, the prototype has shown high performance and the results are consistent with predictions from numerical modelling. Magnetocaloric properties of the Gd spheres were obtained experimentally and implemented in a one-dimensional numerical AMR model that includes also the parasitic losses from the prototype. The temperature span for a thermal load of 200 W as a function of frequency was measured and modelled. Moreover, the temperature span dependence on the cooling capacity as a function of cycle frequency was determined. It was found that thermal losses increase as the frequency increases. Therefore, a detailed study of these parasitic losses was carried out experimentally and numerically.

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Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Federal University of Santa Catarina
Contributors: Lozano, J., Engelbrecht, K., Bahl, C., Nielsen, K. K., Barbosa Jr., J., Prata, A., Pryds, N.
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Experimental results for a novel rotary active magnetic regenerator

Active magnetic regenerator (AMR) refrigerators represent an alternative to vapor compression technology and have great potential in realizing cooling devices with high efficiency, which are highly desirable for a broad range of applications. The technology relies on the magnetocaloric effect in a solid refrigerant rather than the temperature change that occurs when a gas is compressed/expanded. This paper presents the general considerations for the design and construction of a high frequency rotary AMR device. Experimental results are presented at various cooling powers for a range of operating conditions near room temperature. The device exhibited a no-load temperature span of over 25 K and can absorb a 100 W cooling load at a 20.5 K temperature span.

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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
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Web of Science (2016): Indexed yes
Extraordinary high conductivity in SrTiO$_3$-based oxide heterostructures due to interfacial redox reactions

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Management
Contributors: Chen, Y., Christensen, D., Trier, F., Pryds, N., Linderoth, S.
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Source: dtu
Source-ID: u::6409
Research output: Research › Poster – Annual report year: 2012

High performance magnetocaloric perovskites for magnetic refrigeration
We have applied mixed valance manganite perovskites as magnetocaloric materials in a magnetic refrigeration device. Relying on exact control of the composition and a technique to process the materials into single adjoined pieces, we have observed temperature spans above 9 K with two materials. Reasonable correspondence is found between experiments and a 2D numerical model, using the measured magnetocaloric properties of the two materials as input.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science, University of Zaragoza
Contributors: Bahl, C. R. H., Velazquez, D., Nielsen, K. K., Engelbrecht, K., Andersen, K. B., Bulatova, R., Pryds, N.
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Web of Science (2017): Indexed yes
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Web of Science (2016): Impact factor 3.411
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High-temperature segmented thermoelectric oxide module using p-type Ca$_3$Co$_4$O$_9$ and n-type ZnAlO/CaMn$_{0.95}$Nb$_{0.05}$O$_{3}$ legs

Thermoelectric (TE) power generator using TE materials which directly convert heat into electricity offers a viable environmental friendly technology for waste heat recovery. Recently, TE oxide modules have gained much attraction since they are composed of cheap materials and are stable at high temperatures up to 1200 K, where most of the conventional TE materials based on alloys are often degraded over the time. In this report, oxide TE materials of p-type Ca$_3$Co$_4$O$_9$, n-types ZnAlO, and CaMn$_{0.95}$Nb$_{0.05}$O$_3$ were used to fabricate high temperature TE segmented modules. These oxide materials were prepared by solid-state reaction, followed by a spark plasma sintering technique, and their thermoelectric properties were characterized from 300 to 1200 K. The module performance was first investigated by numerical modeling using the experimental thermoelectric properties data as input parameters. In these calculations, the power generation characteristics were investigated in terms of various n-leg selections (ZnAlO, CaMn$_{0.95}$Nb$_{0.05}$O$_3$, and segmented ZnAlO/CaMn$_{0.95}$Nb$_{0.05}$O$_3$), while the p-leg Ca$_3$Co$_4$O$_9$ was fixed. Based on the model prediction, several modules were fabricated, tested, and compared again with the theoretical calculations. The obtained results are discussed in details and also compared with other reported oxide modules.

Improved Modeling Approaches for Constrained Sintering of Bi-Layered Porous Structures

Shape instabilities during constrained sintering experiment of bi-layer porous and dense cerium gadolinium oxide (CGO) structures have been analyzed. An analytical and a numerical model based on the continuum theory of sintering has been implemented to describe the evolution of bow and densification kinetics in the sintering processes that consists of iso-rate and isothermal phases. The significant influence of weight of the sample (gravity) on the evolution of bow, especially in the isothermal sintering phase, is taken into account. The modeling predictions indicate good agreement with the results of sintering of a bi-layered cerium-gadolinium oxide system in terms of evolution of bow, porosity and thickness.
**Materials Challenges for High Performance Magnetocaloric Refrigeration Devices**

Magnetocaloric materials with a Curie temperature near room temperature have attracted significant interest for some time due to their possible application for high-efficiency refrigeration devices. This review focuses on a number of key issues of relevance for the characterization, performance and implementation of such materials in actual devices. The phenomenology and fundamental thermodynamics of magnetocaloric materials is discussed, as well as the hysteresis behavior often found in first-order materials. A number of theoretical and experimental approaches and their implications are reviewed. The question of how to evaluate the suitability of a given material for use in a magnetocaloric device is covered in some detail, including a critical assessment of a number of common performance metrics. Of particular interest is which non-magnetocaloric properties need to be considered in this connection. An overview of several important materials classes is given before considering the performance of materials in actual devices. Finally, an outlook on further developments is presented.

**General information**

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- Web of Science (2017): Impact factor 21.875
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 12.96 SJR 6.515 SNIP 2.14
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 14.2 SJR 6.219 SNIP 2.546
- Web of Science (2015): Impact factor 15.23
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): CiteScore 15.27 SJR 6.668 SNIP 2.942
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): CiteScore 13.24 SJR 6.006 SNIP 2.949
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): CiteScore 9.64 SJR 5.575 SNIP 2.181
- Web of Science (2012): Impact factor 10.043
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- Web of Science (2011): Impact factor
- ISI indexed (2011): ISI indexed no
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Microstructure and thermoelectric properties of screen-printed thick-films of misfit-layered cobalt oxides with Ag addition

Thermoelectric properties of thick (~60 μm) films prepared by a screen-printing technique using p-type misfit-layered cobalt oxide Ca₃Co₄O₉+δ with Ag addition have been studied. The screen-printed films were sintered in air at various temperatures ranging from 973 K to 1223 K. After each sintering process, crystal and microstructure analyses were carried out to determine the optimal sintering condition. The results show that the thermoelectric properties of pure Ca₃Co₄O₉+δ thick film are comparable to those of cold isostatic pressing (CIP) samples. We found that the maximum power factor was improved by about 67% (to 0.3 mW/m K²) for film with proper silver (Ag) metallic inclusions as compared with 0.18 mW/m K² for pure Ca₃Co₄O₉+δ film under the same sintering condition of 1223 K for 2 h in air.

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Peer-reviewed: Yes

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Scopus rating (2017): CiteScore 1.59 SJR 0.474 SNIP 0.772
Web of Science (2017): Impact factor 1.566
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.754
Web of Science (2016): Impact factor 1.579
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.53 SJR 0.555 SNIP 0.802
Web of Science (2015): Impact factor 1.491
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.82 SJR 0.679 SNIP 1.05
Web of Science (2014): Impact factor 1.798
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.71 SJR 0.71 SNIP 1.094
Web of Science (2013): Impact factor 1.675
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.74 SJR 0.865 SNIP 1.298
Web of Science (2012): Impact factor 1.635
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.66 SJR 0.844 SNIP 1.139
Web of Science (2011): Impact factor 1.466
Modeling the microstructural evolution during constrained sintering

A numerical model able to simulate solid state constrained sintering of a powder compact is presented. The model couples an existing kinetic Monte Carlo (kMC) model for free sintering with a finite element (FE) method for calculating stresses on a microstructural level. The microstructural response to the stress field as well as the FE calculation of the stress field from the microstructural evolution is discussed. The sintering behavior of two powder compacts constrained by a rigid substrate is simulated and compared to free sintering of the same samples. Constrained sintering result in a larger number of pores near the substrate as well as a reorientation of the pores along the direction normal to the substrate. These features are also observed experimentally.
Nanostructured Thermoelectric Oxide Materials for Effective Power Generation from Waste Heat

A large amount of thermal energy that emitted from many industrial processes is available as waste heat. It is difficult to reclaim this heat due to the dispersed nature and relative smallness of its sources. Thermoelectric conversion can offer a very promising method to overcome these difficulties by converting heat directly into electricity. However, the requirements for this task place in the materials are not easily satisfied by the conventional thermoelectric materials. Not only they must possess a high thermoelectric performance, they should also be stable at high temperatures and be composed of nontoxic and low-cost elements, and must be able to be processed and shaped cheaply. Oxides are among the strongest candidate materials for this purpose, and recently they have been intensively investigated and developed [1-5]. In this report, the development progress of two state-of-the-art p-type Ca$_3$Co$_4$O$_{9+\delta}$ and n-type doped-ZnO oxide systems is presented. The thermoelectric generator (TEG) devices based on these oxide materials were fabricated, examined, and demonstrated with various output applications. At a $\Delta T = 500$ K, the maximum output power of our TEG composed of 32 $p$-$n$ couples reached 1W, which is among the best one so far and is enough for a practical application such as phone charge or GPS device (see Fig. 1).

On the origin of metallic conductivity at the interface of LaAlO$_3$/SrTiO$_3$

To determine the origin of the quasi-two-dimensional electron gas formed at the interface between the two complex oxides of LaAlO$_3$ (LAO) and SrTiO$_3$ (STO), various amorphous films of LAO, La$_2$O$_3$, Al$_2$O$_3$, and La$_{7/8}$Sr$_{1/8}$MnO$_3$ (LSMO), were deposited on TiO$_2$-terminated (0 0 1) STO substrates by pulsed laser deposition at room temperature. Metallic interfaces are observed when the over-layers are amorphous LAO, La$_2$O$_3$, or Al$_2$O$_3$, while insulating interfaces are observed when the over-layer is LSMO. The interfacial conductivity of these SrTiO$_3$-based hetero-structures shows strong dependence on both film thickness and oxygen pressure during film growth. The possible origin for the occurrence of metallic interfaces in these complex oxide hetero-structures due to redox reactions at the STO substrate surface is discussed. A thermodynamic criterion for designing either metallic or insulating interfaces between complex oxides is proposed.
Oxides gets environmentally-friendly
A large amount of thermal energy is available from the waste heat associated with many industrial and social activities of mankind. However, it is difficult to reclaim this heat due to the dispersed nature and relative smallness of its sources. Thermoelectric conversion offers a very promising method to overcome these difficulties by converting heat directly into electricity at the source. However, the requirements for the materials are not easily satisfied even by current state-of-the-art thermoelectric materials. Not only must they possess high thermoelectric performance, they must also be stable at high temperatures and be composed of nontoxic and low-cost elements, and must be able to be processed and shaped cheaply. Oxides are among the strongest candidate materials for this purpose. This talk provides an overview of the development on such materials at DTU Energy Conversion. In order for high temperature oxide thermoelectric (TE) modules to become a viable route for power generation, the overall efficiency of these devices must be improved. While most research currently focuses on the enhancement of the thermoelectric properties of the p- and n-type elements of the module, it is also necessary to demonstrate a working oxide module and develop stable interconnects with low contact resistance as well as mechanical and the chemical stability. In this presentation I will also show our latest results on the performance of oxide module made of ZnO doped Al (n-type) and CaCoO 349 (p-type) [1]. In the second part of the presentation I will talk about magnetic cooling/heating. In recent years much effort has been put towards development and improvement of active magnetic regenerator (AMR) refrigerators which represent an alternative to vapor compression technology. This technology has great potential in realizing cooling devices with high efficiency and low global warming potentials, which are highly desirable for a broad range of applications. The technology relies on the magnetocaloric effect in a solid refrigerant rather than the temperature change that occurs when a gas is compressed. This talk presents the general considerations for the design and construction of a high frequency rotary AMR device [2]. Recently we have also clearly showed the potential value of the mixed valence manganese ceramics as magnetocaloric materials for application in devices [3]. The strength of the materials lies in the ability to accurately tune the Curie temperature. The relatively low cost of materials and especially the processing route, compared to conventional materials and processing routes, reduces the price which is otherwise a major obstacle in the way of magnetocaloric applications. Finally, the latest experimental results of our novel rotary magnetic refrigeration device are also presented at various cooling powers for a range of operating conditions near room temperature.

Resistance switching of the interfacial conductance in amorphous SrTiO3 heterostructures

Complex oxides have attracted a lot of interest recently as this class of material exhibits a plethora of remarkable properties. In particular, a great variety of properties is observed in the heterostructure composed of lanthanum aluminate (LaAlO3) and strontium titanate (SrTiO3). For instance, at the interface between the two insulating oxides LaAlO3 and SrTiO3 a high-mobility quasi-two-dimensional electron gas is formed if the thickness of LaAlO3 exceeds a critical value of 3 unit cells. At a thickness of 3 unit cells the interface remains insulating, however, an interface conductance can be induced by an electric field. It has previously been demonstrated that SrTiO3 heterostructures with amorphous LaAlO3 top layers can display interfacial conductivity with similar critical thickness dependence. Here, we report resistance switching of the interfacial conductance for SrTiO3 heterostructures with amorphous LaAlO3 top layers below the critical thickness in various controlled environments.

Strain induced ionic conductivity enhancement in epitaxial Ce0.9Gd0.1O2-δ

Strained epitaxial Ce0.9Gd0.1O2-δ (CGO) thin films are deposited on MgO(001) substrates with SrTiO3 (STO) buffer layers. The strain in CGO epitaxial thin films is induced and controlled by varying the thickness of STO buffer layers. The induced strain is found to significantly enhance the in-plane ionic conductivity in CGO epitaxial thin films. The ionic conductivity is found to increase with decrease in buffer layer thickness. The tailored ionic conductivity enhancement is explained in terms of close relationships among epitaxy, strain, and ionic conductivity.
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  BFI (2017): BFI-level 2
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  Web of Science (2017): Impact factor 3.495
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
  Web of Science (2016): Impact factor 3.411
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  BFI (2015): BFI-level 2
  Scopus rating (2015): CiteScore 2.47 SJR 1.499 SNIP 1.226
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  Web of Science (2014): Impact factor 3.302
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): CiteScore 3.77 SJR 2.146 SNIP 1.633
  Web of Science (2013): Impact factor 3.515
  ISI indexed (2013): ISI indexed yes
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  BFI (2012): BFI-level 2
  Scopus rating (2012): CiteScore 3.76 SJR 2.57 SNIP 1.739
  Web of Science (2012): Impact factor 3.794
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): CiteScore 4.04 SJR 2.814 SNIP 1.917
  Web of Science (2011): Impact factor 3.844
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 2.92 SNIP 1.775
  Web of Science (2010): Impact factor 3.841
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 2.826 SNIP 1.834
  Web of Science (2009): Indexed yes
  BFI (2008): BFI-level 2
  Scopus rating (2008): SJR 2.894 SNIP 1.82
  Web of Science (2008): Indexed yes
  Scopus rating (2007): SJR 3.012 SNIP 1.916
  Web of Science (2007): Indexed yes
  Web of Science (2006): Indexed yes
Structure useful for producing a thermoelectric generator, thermoelectric generator comprising same and method for producing same

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Contributors: Van Nong, N., Pryds, N., Bahl, C., Smith, A., Linderoth, S.
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Publication information
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Source: dtu
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Research output: Research › Patent – Annual report year: 2013

The creation of two-dimensional electron gases in SrTiO$_3$-based complex oxide heterostructures by interface redox reactions

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Contributors: Chen, Y., Trier, F., Christensen, D., Pryds, N.
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WOE19_abstract_yunzhong.pdf
The influence of non-magnetocaloric properties on the AMR performance
The performance of Active Magnetic Regenerators (AMR) does not depend solely on the magnetocaloric effect of their constituents. Rather, it depends on several additional parameters, including, magnetic field, geometry (hydraulic diameter, cross-sectional area, regenerator length etc.), thermal properties (conductivity, specific heat and mass density) and operating parameters (utilization, frequency, number of transfer units etc.). In this paper we focus on the influence of three parameters on regenerator performance: 1) Solid thermal conductivity, 2) magnetostatic demagnetization and 3) flow maldistribution due to geometrically non-uniform regenerators.

It is shown that the AMR performance is optimal at an intermediate value of the solid thermal conductivity for many operating conditions. The magnetostatic demagnetization is shown to have a significant influence on the AMR performance, giving a strong dependence on the orientation of the applied field and the regenerator geometry. Finally, the flow maldistribution of non-uniform regenerator geometries is found to degrade the AMR performance even at minor deviations from perfectly homogeneous regenerator matrices.

The Influence of Spark Plasma Sintering Temperature on the Microstructure and the Thermoelectric Properties of Al, Ga dually-doped ZnO
Al, Ga dually-doped ZnO was prepared by spark plasma sintering with different sintering temperatures. The microstructural evolution and thermoelectric properties of the samples were investigated in detail. The samples with a sintering temperature above 1223K obtained higher relative densities and better electrical properties compared with the sample sintered at 1073K. These results were supported by solid-state-reaction completion rate which suggested that the sintering temperature above 1223K would be preferable for the complete solid state reaction of the samples. The sintering mechanism of ZnO particles and microstructure evolutions at different sintering temperatures were investigated by the simulation of the self-Joule-heating effect of the individual particles.

The Influence of α- and γ-Al₂O₃ Phases on the Thermoelectric Properties of Al-doped ZnO

The Kinetics, Stability and Thermal Contact Resistance of Nickel-Ca$_3$Co$_4$O$_9$ Interfaces Formed by Spark Plasma Sintering

Incorporating oxide thermoelectric (TE) materials in TE power generation modules necessitates the study of the interfaces between the oxide TE elements and the interconnect materials used to deliver current between them. In this study, interfaces between pure nickel and undoped calcium cobaltate (Ca$_3$Co$_4$O$_9$) have been formed directly by spark plasma sintering (SPS). An intermediate NiO phase is formed during the SPS processes, which grows during post heating with Co entering from the cobaltate side to form a graded Ni$_{1-x}$Co$_x$O interfacial layer. The electrical and thermal transport across these interfaces, as well as the long term chemical stability of the intermediate layers, have been studied and are discussed herein.

Thermoelectric Properties and Microstructure of Modified Novel Complex Cobalt Oxides Sr$_3$RECo$_4$O$_{10.5}$ (RE = Y, Gd)

We report on the high-temperature thermoelectric properties and microstructure of modified novel complex cobalt oxides Sr$_3$RECo$_4$O$_{10.5}$ (RE = Y, Gd), in which the Sr- and Co-sites are partly substituted by Ca and Ga, respectively. We have found that the sample with RE = Gd shows a significant higher electrical conductivity (sigma) than the RE = Y sample, while their Seebeck coefficients (S) remain almost the same over the whole measured temperature range. With Ga substituting for Co, S is enhanced and further increased by the dually doping with Ca at the Sr-site, leading to an improvement of the thermoelectric power factor (sigma S$^{-2}$). At 1150 K, the highest sigma S$^{-2}$ value attains for the Sr$_2$CaGdCo$_3.9$Ga$_0.1$O$_{10.5}$ sample about 60 mu Wm$^{-1}$K$^{-2}$, which is 8 times larger than the Sr$_3$GdCo$_4$O$_{10.5}$ counterpart. Interestingly, although microstructure shows a clear evolution of the grains for the Ga and Ca doped-sample resulting in a substantial decrease in porosity, its thermal diffusivity exhibits a lower value then the non-doped one, particularly in high temperature region. © 2012 American Institute of Physics
The sintering behavior of close-packed spheres
The sintering behavior of close-packed spheres is investigated using a numerical model. The investigated systems are the body-centered cubic (bcc), face-centered cubic (fcc) and hexagonal close-packed spheres (hcp). The sintering behavior is found to be ideal, with no grain growth until full density is reached for all systems. During sintering, the grains change shape from spherical to tetrakaidecahedron, similar to the geometry analyzed by Coble [R.L. Coble, J. Appl. Phys. 32 (1961) 787].

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Mixed Conductors, Sandia National Laboratories
Contributors: Bjørk, R., Tikare, V., Frandsen, H. L., Pryds, N.
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Publication information
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Volume: 67
Issue number: 1
Design concepts for a continuously rotating active magnetic regenerator

Design considerations for a prototype magnetic refrigeration device with a continuously rotating AMR are presented. Building the active magnetic regenerator (AMR) from stacks of elongated plates of the perovskite oxide material La0.67Ca0.33−xSrxMn1.05O3, gives both a low pressure drop and allows grading of the Curie temperature along the plates. This may be accomplished by a novel technique where a compositionally-graded material is tape cast in one piece. The magnet assembly is based on a novel design strategy, to create alternating high- and low magnetic field regions within a magnet assembly. Focus is on maximising the magnetic field in the high field regions but also, importantly, minimising the flux in the low field regions. The design is iteratively optimised through 3D finite element magnetostatic modelling.

General information
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Contributors: Bahl, C. R. H., Engelbrecht, K., Bjørk, R., Eriksen, D., Smith, A., Nielsen, K. K., Pryds, N.
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Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.44 SJR 1.349 SNIP 1.532
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Non-Uniform Heat Transfer in Thermal Regenerators

This thesis presents investigations on the heat transfer in complex heat exchangers in general and in regenerative heat exchangers (regenerators) in particular. The motivation for this work is a result of inconsistencies observed in the results from a series of experiments on active magnetic regenerators (AMRs) with parallel plates. The results suggest that random variations in the regenerator geometries cause maldistributed fluid flow inside the regenerators, which affects the regenerator performance. In order to study the heat transfer processes in regenerators with non-uniform geometries, a numerical model, which simulates a single-blow operation in a parallel-plate regenerator, was developed and used to model the heat transfer under various conditions. In addition to the modeling of the heat transfer, a series of experiments on passive regenerators with non-uniform, but precisely controlled, geometries was performed. The objective of performing these experiments was in part to evaluate the direct applicability of the model, which only simulates one half
of the regenerator cycle, to a practical situation where the regenerator is running con- tinuously by comparing the results gained. Additionally, the experiments gave real comparative results, whereas the model to a certain degree more served to provide insight to the heat transfer processes taking place inside the regenera- tors, something that would be - if not impossible - then highly impractical to do experimentally. It has been found that non-uniformity in the plate spacings of non-uniform regenerators can have a significant impact on the regenerator effectiveness, particularly for regenerators with small plate spacings. The observed reduc- tions in effectiveness have furthermore been found to alter the optimim plate spacing, and decreasing the plate spacing beyon- d a certain point can even hurt the performance. Inter-channel heat transfer effects - or thermal cross-talk - have also been in- vestigated and the results show that not only the size of the plate spacings, but also their mutual order, can affect the heat transfer significantly.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermal Energy, Department of Mechanical Engineering
Contributors: Jensen, J. B., Pryds, N., Bahl, C. R. H., Elmegaard, B.
Publication date: Oct 2011

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Publisher: Technical University of Denmark (DTU)
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Developing New Electrolytes Materials and Methods for the Manufacture of Nanostructured Electrolytes for Low Temperature SOFC Operating Around 400°C

General information
State: Published
Contributors: Janik, K. A., Pryds, N., Linderoth, S., Kuhn, L. T.
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Research output: Research › Ph.D. thesis – Annual report year: 2011

A Magnetic Assembly, a Fluid-Flow Assembly and an Indicator
The invention provides a magnetic assembly, the assembly comprising: a magnet (4); and a ferromagnetic component (6) having at least two regions of different Curie temperature, the magnet (4) and the ferromagnetic component being movable with respect to each other in dependence on the temperature of the ferromagnetic component (6).

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Contributors: Bahl, C. R. H., Smith, A., Pryds, N.
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Publication information
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Patent number: US 20110030826
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Bibliographical note
A Monolithic Perovskite Structure for Use as a Magnetic Regenerator

A La0.67Ca0.26Sr0.07Mn1.05O3 (LCSM) perovskite was prepared for the first time as a ceramic monolithic regenerator used in a regenerative magnetic refrigeration device. The parameters influencing the extrusion process and the performance of the regenerator, such as the nature of the monolith paste and the influence of the sintering on the adiabatic temperature change, were investigated. Comparisons between the extruded monolithic structure before and after the sintering showed that an increase of the adiabatic temperature change was seen after the sintering. Furthermore, calculations show that the performance of the monolithic structure is potentially superior to a parallel plate regenerator, indicating the potential cost and structural benefit of using such structure, i.e. a mechanically stable ceramic thin wall structure, which can be produced in one processing step.
Analysis of Key Factors Controlling Sintering of Dense and Porous CGO Bi-layers

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Electroceramics, Ceramic processing, San Diego State University
Contributors: Tadesse Molla, T., Frandsen, H. L., Esposito, V., Bjerk, R., Foghmoes, S. P. V., Olevsky, E., Pryds, N.
Publication date: 2011
Peer-reviewed: No
Analysis of single blow effectiveness in non-uniform parallel plate regenerators
Non-uniform distributions of plate spacings in parallel plate regenerators have been found to induce loss of performance. In this paper, it has been investigated how variations of three geometric parameters (the aspect ratio, the porosity, and the standard deviation of the plate spacing) affects this loss in a single blow model of a parallel-plate regenerator. Simple analytical functions for the magnitude and the time scale of the reduction of performance are presented and compared to numerical results.

General information
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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermal Energy, Department of Mechanical Engineering
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Web of Science (2017): Impact factor 3.891
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.75 SJR 1.605 SNIP 2.013
Web of Science (2016): Impact factor 3.458
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.09 SJR 1.733 SNIP 1.905
Web of Science (2015): Impact factor 2.857
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.97 SJR 1.584 SNIP 1.973
Web of Science (2014): Impact factor 2.383
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.38 SJR 0.88 SNIP 2.134
Web of Science (2013): Impact factor 2.522
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.79 SJR 1.626 SNIP 2.121
Web of Science (2012): Impact factor 2.315
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.04 SJR 1.066 SNIP 1.951
Web of Science (2011): Impact factor 2.407
An experimental study of passive regenerator geometries

Active magnetic regenerative (AMR) systems are being investigated because they represent a potentially attractive alternative to vapor compression technology. The performance of these systems is dependent on the heat transfer and pressure drop performance of the regenerator geometry. Therefore this article studies the effects of regenerator geometry on performance for flat plate regenerators. This paper investigates methods of improving the performance of flat plate regenerators for use in AMR systems and studies how manufacturing variation affects regenerator performance. In order to eliminate experimental uncertainty associated with magnetocaloric material properties, all regenerators are made of aluminum. The performance of corrugated plates and dimpled plates are compared to traditional flat plate regenerators for a range of cycle times and utilizations. Each regenerator is built using 18 aluminum plates with a 0.4 mm thickness, which allows their performance to be compared directly.

General information
State: Published
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Contributors: Engelbrecht, K., Nielsen, K. K., Pryds, N.
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Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
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BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.44 SJR 1.349 SNIP 1.532
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.6 SJR 1.619 SNIP 2.086
Web of Science (2014): Impact factor 2.241
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.25 SJR 1.422 SNIP 1.944
Web of Science (2013): Impact factor 1.702
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.09 SJR 1.386 SNIP 1.893
Web of Science (2012): Impact factor 1.793
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.2 SJR 1.272 SNIP 2.129
Web of Science (2011): Impact factor 1.817
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.355 SNIP 1.789
Web of Science (2010): Impact factor 1.439
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.565 SNIP 1.972
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.282 SNIP 1.734
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.848 SNIP 1.629
Scopus rating (2006): SJR 1.497 SNIP 1.643
Scopus rating (2005): SJR 1.384 SNIP 1.682
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.174 SNIP 1.916
Scopus rating (2003): SJR 1.222 SNIP 1.507
Scopus rating (2002): SJR 1.642 SNIP 1.809
Scopus rating (2001): SJR 1.9 SNIP 1.869
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.816 SNIP 1.314
Scopus rating (1999): SJR 0.809 SNIP 1.214

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Anomalously high thermoelectric power factor in epitaxial ScN thin films

Thermoelectric properties of ScN thin films grown by reactive magnetron sputtering on Al2O3(0001) wafers are reported. X-ray diffraction and elastic recoil detection analyses show that the composition of the films is close to stoichiometry with trace amounts (~1 at.% in total) of C, O, and F. We found that the ScN thin-film exhibits a rather low electrical resistivity of ~2.94 μΩm, while its Seebeck coefficient is approximately ~−86 μV/K at 800 K, yielding a power factor of ~2.5 × 10⁻³ W/mK². This value is anomalously high for common transition-metal nitrides. © 2011 American Institute of Physics
Charge modulated interfacial conductivity in SrTiO3-based oxide heterostructures

When depositing amorphous SrTiO3 (STO) films on crystalline STO substrates by pulsed laser deposition, metallic interfaces are observed, though both materials are band-gap insulators. The interfacial conductivity exhibits strong dependence on oxygen pressure during film growth, which is closely related to the STO plasma expansion in the background gas of oxygen. By controlling the charge balance in the STO plasma with an external bias, V-bias, of -10 V
Determining the minimum mass and cost of a magnetic refrigerator

An expression is determined for the mass of the magnet and magnetocaloric material needed for a magnetic refrigerator and these are determined using numerical modeling for both parallel plate and packed sphere bed regenerators as function of temperature span and cooling power. As magnetocaloric material Gd or a model material with a constant adiabatic temperature change, representing an infinitely linearly graded refrigeration device, is used. For the magnet a maximum figure of merit magnet or a Halbach cylinder is used. For a cost of $40 and $20 per kg for the magnet and magnetocaloric material, respectively, the cheapest 100 W parallel plate refrigerator with a temperature span of 20 K using Gd and a Halbach magnet has 0.8 kg of magnet, 0.3 kg of Gd and a cost of $35. Using the constant material reduces this cost to $25. A packed sphere bed refrigerator with the constant material costs $7. It is also shown that increasing the operation frequency reduces the cost. Finally, the lowest cost is also found as a function of the cost of the magnet and magnetocaloric material.

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Scopus rating (2017): CiteScore 3.46 SJR 1.471 SNIP 1.888
Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.44 SJR 1.349 SNIP 1.532
Web of Science (2015): Indexed yes
Enhanced electrochemical performance of the solid oxide fuel cell cathode using Ca₃Co₄O₉+δ

This paper reports on the electrochemical performance of an SOFC cathode for potential use in intermediate-temperature solid oxide fuel cells (IT-SOFCs) using the oxygen non-stoichiometric misfit-layered cobaltite Ca₃Co₄O₉+δ or composites of Ca₃Co₄O₉+δ with Ce₀.₉Gd₀.₁O₁.₉₅ (CGO/Ca₃Co₄O₉+δ). Electrochemical impedance spectroscopy revealed that symmetric cells with an electrode of pure Ca₃Co₄O₉+δ exhibit a cathode polarization resistance (Rp) of 12.4 Ω cm², at 600 °C in air. Strikingly, Rp of the composite CGO/Ca₃Co₄O₉+δ with 50 vol.% CGO was reduced by a factor of 19 (i.e.
Rp = 0.64 Ω cm²), the lowest value reported so far for the Ca₃Co₄O₉ family of compounds. These findings together with the reported thermal expansion coefficient, good compatibility with CGO and chemical durability of this material suggest that it is a promising candidate cathode for IT-SOFCs.

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Organisations: Risø National Laboratory for Sustainable Energy, Electroceramics, Fuel Cells and Solid State Chemistry Division, Thermo Ceramics

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- 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
- Web of Science (2016): Indexed yes
- 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
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): CiteScore 5.04 SJR 2.282 SNIP 2.006
- Web of Science (2012): Impact factor 4.675
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): CiteScore 5.13 SJR 2.227 SNIP 2.172
- Web of Science (2011): Impact factor 4.951
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.294 SNIP 1.972
- Web of Science (2010): Impact factor 4.29
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
Enhancement of the thermoelectric performance of p-type layered oxide Ca$_3$Co$_4$O$_9+$ through heavy doping and metallic nanoinclusions

An effective way to improve the thermoelectric performance (ZT) of layered structured oxide materials by carefully choosing heavy ion doping and introducing metallic nanoinclusions is proposed. A p-type oxide material with remarkable highly improved ZT is successfully fabricated using this approach. Long-term durability at high temperature testing confirms this material is a very promising p-type material for high temperature power generation.

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Contributors: Van Nong, N., Pryds, N., Linderoth, S., Ohtaki, M.
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Web of Science (2017): Impact factor 2.227
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 17.79
Web of Science (2016): Impact factor 1.333
Web of Science (2016): Indexed yes
Epitaxial growth of atomically flat gadolinia-doped ceria thin films by pulsed laser deposition

Epitaxial growth of Ce0.8Gd0.2O2(CGO) films on (001) TiO2-terminated SrTiO3 substrates by pulsed laser deposition was investigated using in situ reflective high energy electron diffraction. The initial film growth shows a Stransky-Krastanov growth mode. However, this three-dimensional island formation is replaced by a two-dimensional island nucleation during further deposition, which results in atomically smooth CGO films. The obtained high-quality CGO films may be attractive for the electrolyte of solid-oxide fuel cells operating at low temperature.

General information
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Contributors: Chen, Y., Pryds, N., Schou, J., Linderoth, S.
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Extraordinarily high conductivity at interfaces of ZrO2:Y2O3/SrTiO3 heterostructures: origin and perspective

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Contributors: Chen, Y., Christensen, D., Trier, F., Pryds, N., Smith, A., Linderoth, S.
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Research output: Research › Poster – Annual report year: 2011

Growth and thermoelectric properties of FeSb2 films produced by pulsed laser deposition
Thermoelectric FeSb2 films were produced by pulsed laser deposition on silica substrates in a low-pressure Ar environment. The growth conditions for near phase-pure FeSb2 films were confirmed to be optimized at a substrate temperature of 425°C, an Ar pressure of 2 Pa, and deposition time of 3 h by abrating specifically prepared compound targets made of Fe and Sb powders in atomic ratio of 1:4. The thermoelectric transport properties of FeSb2 films were investigated. Pulsed laser deposition was demonstrated as a method for production of good-quality FeSb2 films.

General information
State: Published
Organisations: Optical Microsensors and Micromaterials, Department of Photonics Engineering, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Aarhus University, Max Planck Institute
Contributors: Sun, Y., Canulescu, S., Sun, P., Steglich, F., Pryds, N., Brummerstedt Iversen, B.
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Publication date: 2011
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Heavy ions doping coupled with metallic nanoinclusions: An effective way to improve the thermoelectric performance of p-type layered cobalt oxide materials

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Contributors: Van Nong, N., Pryds, N., Linderoth, S., Ohtaki, M.
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High-temperature Thermoelectric and Microstructural Characteristics of Ga Substituted on the Co-site in Cobalt-based Oxides
The effects of Ga substitution on the Co-site on the high-temperature thermoelectric properties and microstructure are investigated for the misfitlayered Ca3Co4O9 and the complex perovskite-related Sr3RECo4O10.5 (RE = rare earth) cobalt-based oxides. For both systems, substitution of Ga for Co results in a simultaneous increase in the Seebeck coefficient (S) and the electrical conductivity (σ), and the influence is more significant in the high temperature region. The power factor (S 2 σ) is thereby remarkably improved by Ga substitution, particularly at high temperatures. Texture factor calculations using x-ray diffraction pattern data for pressed and powder samples reveal that the Ga-doped samples are highly textured. Microstructure observed by scanning electron microscopy shows very well-crystallized grains for the samples with Ga substitution for Co. Among the Ga-doped samples, Ca3Co3.95Ga0.05O9 shows the best ZT value of 0.45 at 1200 K, which is about 87.5% higher than the nondoped one, a considerable improvement.

General information
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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Hakodate National College of Technology, Kyushu University
Contributors: Van Nong, N., Yanagiya, S., Sonne, M., Pryds, N., Ohtaki, M.
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BFI (2017): BFI-level 1
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.754
Web of Science (2016): Impact factor 1.579
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.53 SJR 0.555 SNIP 0.802
Web of Science (2015): Impact factor 1.491
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.82 SJR 0.679 SNIP 1.05
Web of Science (2014): Impact factor 1.798
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.71 SJR 0.71 SNIP 1.094
Web of Science (2013): Impact factor 1.675
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.74 SJR 0.865 SNIP 1.298
Web of Science (2012): Impact factor 1.635
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.66 SJR 0.844 SNIP 1.139
Web of Science (2011): Impact factor 1.466
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.773 SNIP 1.035
Web of Science (2010): Impact factor 1.421
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.907 SNIP 1.133
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.858 SNIP 0.953
Scopus rating (2007): SJR 0.879 SNIP 1.058
Scopus rating (2006): SJR 1.028 SNIP 1.222
Scopus rating (2005): SJR 1.13 SNIP 1.199
Scopus rating (2004): SJR 1.097 SNIP 1.184
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.189 SNIP 1.145
Scopus rating (2002): SJR 1.37 SNIP 1.23
Scopus rating (2001): SJR 1.279 SNIP 1.175
Scopus rating (2000): SJR 1.462 SNIP 0.978
Scopus rating (1999): SJR 1.365 SNIP 0.938
Original language: English
Keywords: Magnetic refrigeration
Electronic versions:
Van nong paper2.pdf
DOIs:
10.1007/s11664-011-1524-1
Source: orbit
Source-ID: 275374
Research output: Research - peer-review › Journal article – Annual report year: 2011
Imposed quasi-layer-by-layer homoepitaxial growth of SrTiO3 films by large area pulsed laser deposition

The homoepitaxial growth of SrTiO3 (STO) films was investigated by a large-area pulsed laser deposition (PLD), which was in-situ monitored by a high pressure reflective high energy electron diffraction. By combining a conventionally continuous film deposition with a followed interval relaxation, a persistent layer-by-layer (LBL) film growth of more than 100 unit cells STO films was achieved. This interrupted PLD technique could realize persistent LBL film growth at any laser frequency between 1 and 10 Hz and provides an effective way to fabricate high quality complex oxide films on unit cell scale.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Chen, Y., Pryds, N.
Pages: 6330-6333
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Thin Solid Films
Volume: 519
Issue number: 19
ISSN (Print): 0040-6090
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.91 SJR 0.617 SNIP 0.864
Web of Science (2017): Impact factor 1.939
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.83 SJR 0.639 SNIP 0.881
Web of Science (2016): Impact factor 1.879
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.84 SJR 0.68 SNIP 0.923
Web of Science (2015): Impact factor 1.761
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.94 SJR 0.725 SNIP 1.075
Web of Science (2014): Impact factor 1.759
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2 SJR 0.814 SNIP 1.195
Web of Science (2013): Impact factor 1.867
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.86 SJR 0.897 SNIP 1.153
Web of Science (2012): Impact factor 1.604
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.13 SJR 0.995 SNIP 1.323
Web of Science (2011): Impact factor 1.89
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Improving Magnet Designs With High and Low Field Regions

A general scheme for increasing the difference in magnetic flux density between a high and a low magnetic field region by removing unnecessary magnet material is presented. This is important in, e.g., magnetic refrigeration where magnet arrays have to deliver high field regions in close proximity to low field regions. Also, a general way to replace magnet material with a high permeability soft magnetic material where appropriate is discussed. As an example, these schemes are applied to a two dimensional concentric Halbach cylinder design resulting in a reduction of the amount of magnet material used by 42% while increasing the difference in flux density between a high and a low field region by 45%.
Magnetic refrigeration at room temperature - from magnetocaloric materials to a prototype

Based on the magnetocaloric effect, magnetic refrigeration at room temperature has for the past decade been a promising, environmentally friendly new energy technology predicted to have a significantly higher efficiency than the present conventional methods. However, so far only a few prototype refrigeration machines have been presented worldwide and there are still many scientific and technological challenges to be overcome. We report here on the MagCool project, which spans all the way from basic materials studies to the construction of a prototype. Emphasis has been on ceramic magnetocaloric materials, their shaping and graded composition for technological use. Modelling the performance of a permanent magnet with optimum use of the flux and relatively low weight, and designing and constructing a prototype continuous magnetic refrigeration device have also been major tasks in the project.

General information
State: Published
Contributors: Kuhn, L. T., Pryds, N., Bahl, C. R. H., Smith, A.
Pages: 012082
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Physics: Conference Series (Online)
Volume: 303
Issue number: 1
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.48 SJR 0.241 SNIP 0.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.35 SJR 0.252 SNIP 0.374
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.32 SJR 0.264 SNIP 0.352
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.25 SJR 0.245 SNIP 0.293
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.33 SJR 0.293 SNIP 0.387
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.43 SJR 0.293 SNIP 0.356
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.288 SNIP 0.351
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Metallic and insulating interfaces of amorphous SrTiO₃-based oxide heterostructures

General information
State: Published
Publication date: 2011

Host publication information
Title of host publication: Abstracts
Electronic versions: MAMA workshop[1].pdf
Source: orbit
Source-ID: 313815
Research output: Research › Conference abstract in proceedings – Annual report year: 2011

Metallic and Insulating Interfaces of Amorphous SrTiO₃-Based Oxide Heterostructures
The conductance confined at the interface of complex oxide heterostructures provides new opportunities to explore nanoelectronic as well as nanionic devices. Herein we show that metallic interfaces can be realized in SrTiO₃-based heterostructures with various insulating overlayers of amorphous LaAlO₃, SrTiO₃, and yttria-stabilized zirconia films. On the other hand, samples of amorphous La₇/₈Sr₈/₈MnO₃ films on SrTiO₃ substrates remain insulating. The interfacial conductivity results from the formation of oxygen vacancies near the interface, suggesting that the redox reactions on the surface of SrTiO₃ substrates play an important role.

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Pages: 3774-3778
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Nano Letters
Volume: 11
Issue number: 9
ISSN (Print): 1530-6984
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Microstructure and thermoelectric properties of misfit-layered cobalt oxides with metallic nanoinclusions prepared by a printing technique
Nanostructured PLD-grown gadolinia doped ceria: Chemical and structural characterization by transmission electron microscopy techniques

The morphology as well as the spatially resolved elemental and chemical characterization of 10 mol% gadolinia doped ceria (CGO10) structures prepared by pulsed laser deposition (PLD) technique are investigated by scanning transmission electron microscopy accompanied with electron energy loss spectroscopy and energy dispersive X-ray spectroscopy. A dense, columnar and structurally inhomogeneous CGO10 film, i.e. exhibiting grain size refinement across the film thickness, is obtained in the deposition process. The cerium M4,5 edges, used to monitor the local electronic structure of the grains, indicate apparent variation of the ceria valence state across and along the film. No element segregation to the grain boundaries is detected. These results are discussed in the context of solid oxide fuel cell applications.
Pulsed laser deposition growth of FeSb2 films for thermoelectric applications

FeSb2 films were produced in a low-pressure Ar environment by pulsed laser deposition at 355 nm. The influence of growth parameters such as substrate temperature, Ar pressure and deposition time on the growth of FeSb2 films was studied. Nearly phase-pure FeSb2 films with thicknesses of 100–400 nm were produced at 425 °C with an Ar pressure of 1.5–2 Pa. Thermal transport and Hall measurements were performed to explore the thermoelectric transport properties of the FeSb2 films. A maximum thermopower of 120 μVK−1 at 40 K was obtained. In general it is highly important to understand the growth properties of FeSb2 films if they are to eventually reach thermoelectric applications at cryogenic temperatures.
Recent Progress in Nanostructured Oxide TE Materials for Power Generation at High Temperatures

Thermoelectric (TE) materials, which can convert waste heat into electricity, could play an important role in a global sustainable energy solution and environmental problems. Metal oxides have been considered as potential TE materials for power generation that can operate at high temperatures on the basis of their advantages over chemical and thermal robustness, nontoxic and cheap composed elements. Among oxide materials, layered-cobalites such as NaCo2O4 and Ca3Co4O9 have recently attracted much attention due to their unusual high TE figure of merit with single crystals, ZT ≈ 1 at 1000 K (ZT = S²σT/κ , where S, σ, T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively). We have fabricated high-quality oxide TE materials based on Ca3Co4O9 by optimizing the method for synthesis, modifying the compositions and by nanostructuring. This report will focus on the high temperature TE properties of heavy ions doping nanostructured Ca3Co4O9 oxides, which exhibit promising ZT, implying suitable polycrystalline oxide TE materials for power generation from waste heat.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Fuel Cells and Solid State Chemistry Division. Management, Kyushu University, Hanoi University of Science and Technology
Publication date: 2011
Peer-reviewed: No
Event: Abstract from 5th International Workshop on Advanced Materials Science and Nanotechnology, Nanoi (VN), 9-12 Nov, .
Keywords: Magnetic refrigeration
Source: orbit
Source-ID: 275399
Research output: Research › Conference abstract for conference – Annual report year: 2011

Review on numerical modeling of active magnetic regenerators for room temperature applications

The active magnetic regenerator (AMR) is an alternative refrigeration cycle with a potential gain of energy efficiency compared to conventional refrigeration techniques. The AMR poses a complex problem of heat transfer, fluid dynamics and magnetic fields, which requires detailed and robust modeling. This paper reviews the existing numerical modeling of room temperature AMR to date. The governing equations, implementation of the magnetocaloric effect (MCE), fluid flow and magnetic field profiles, thermal conduction etc. are discussed in detail as is their impact on the AMR cycle. Flow channeling effects, hysteresis, thermal losses and demagnetizing fields are discussed and it is concluded that more detailed modeling of these phenomena is required to obtain a better understanding of the AMR cycle.

General information
State: Published
Pages: 603-616
Publication date: 2011
Structural, magnetic and magnetocaloric properties of Heusler alloys Ni50Mn38Sb12 with boron addition

We report on the structural, magnetic and magnetocaloric properties of the Ni50Mn38Sb12Bx alloys in terms of boron addition with x=1, 3 and 5. We have found that both the paramagnetic–ferromagnetic austenitic transition (TC) and the ferromagnetic–antiferromagnetic martensitic transition (TM) are sensitively influenced by the boron addition: TC tends to increase, while TM decreases with increasing boron concentration. Temperature dependent X-ray diffraction in the range of 200–500K clearly shows an evolution of the structural transformation from orthorhombic to cubic structure phase transition on heating for the x=1 and 3 samples. Strikingly, the addition of boron atoms into the lattice favours the ferromagnetic ordering relatively to the antiferromagnetic arrangement below TM. This consequently affects on the magneto-structural transition as well as on the size of magnetocaloric effect.
The effects of thermal annealing on the structure and the electrical transport properties of ultrathin gadolinia-doped ceria films grown by pulsed laser deposition

Ultrathin crystalline films of 10 mol% gadolinia-doped ceria (CGO10) are grown on MgO (100) substrates by pulsed laser deposition at a moderate temperature of 400°C. As-deposited CGO10 layers of approximately 4 nm, 14 nm, and 22 nm thickness consist of fine grains with dimensions ≤∼11 nm. The films show high density within the thickness probed in the X-ray reflectivity experiments. Thermally activated grain growth, density decrease, and film surface roughening, which may result in the formation of incoherent CGO10 islands by dewetting below a critical film thickness, are observed upon heat treatment at 400°C and 800°C. The effect of the grain coarsening on the electrical characteristics of the layers is investigated and discussed in the context of a variation of the number density of grain boundaries. The results are evaluated with regard to the use of ultrathin CGO10 films as seeding templates for the moderate temperature growth of thick solid electrolyte films with improved oxygen transport properties.

General information
State: Published
Organisations: Microstructures and Interfaces, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics, Ceramic processing, Fuel Cells and Solid State Chemistry Division. Management, Optical Microsensors and Micromaterials, Department of Photonics Engineering, Paul Scherrer Institute
Pages: 845-850
Thermoelectric properties and microstructure of modified novel complex cobalt oxides Sr3RECo4O10.5 (RE = Y and Gd): Abstract of poster presentation

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Van Nong, N., Pryds, N.
Publication date: 2011
Peer-reviewed: No
Event: Abstract from 9th European Conference on Thermoelectrics, Thessaloniki, Greece.
Keywords: Magnetic refrigeration
Electronic versions:
Nong_et_al_ECT2011_abstract.pdf
Source: orbit
Source-ID: 280202
Research output: Research › Conference abstract for conference – Annual report year: 2011

Thermoelectric Properties and Microstructure of Modified Novel Complex Cobalt Oxides Sr3RECo4O10.5 (RE = Y, Gd)

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Van Nong, N., Pryds, N.
Pages: B_66_P
Publication date: 2011

Host publication information
Title of host publication: Proceedings
Publisher: American Institute of Physics
Source: orbit
Source-ID: 285175
Research output: Research › Article in proceedings – Annual report year: 2011

Thermoelectric properties of ScN thin films

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thin Film Physics Division, Department of Physics, Chemistry, and Biology (IFM), (SE)
Thermoelectric properties of SnO2-based ceramics doped with Nd, Hf or Bi

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Hakodate National College of Technology
Contributors: Yanagiya, S., Van Nong, N., Sonne, M., Pryds, N.
Pages: B_55_P
Publication date: 2011

Thermoelectric Properties of SnO2 Ceramics Doped with Sb and Zn
Polycrystalline SnO2-based samples (Sn0.97−x Sb0.03Zn xO2, x = 0, 0.01, 0.03) were prepared by solid-state reactions. The thermoelectric properties of SnO2 doped with Sb and Zn were investigated from 300 K to 1100 K. X-ray diffraction (XRD) analysis revealed all XRD peaks of all the samples as identical to the rutile structure, except for the x = 0.03 sample, which had a small amount of Zn2SbO4 as a secondary phase. We found that the power factor of the x = 0.03 sample was significantly improved due to the simultaneous increase in the electrical conductivity and the Seebeck coefficient. A power factor value of ∼2 × 10−4 W m−1 K−2 was obtained for the x = 0.03 sample at 1060 K, 126% higher than that for the undoped sample.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Hakodate National College of Technology
Contributors: Yanagiya, S., Van Nong, N., Xu, J. J., Sonne, M., Pryds, N.
Pages: 674-677
Publication date: 2011
Peer-reviewed: Yes
Designing a magnet for magnetic refrigeration

This thesis investigates the design and optimization of a permanent magnet assembly for use in a magnetic refrigeration device. The heart of magnetic refrigeration is the adiabatic temperature change in the magnetocaloric material which is caused by the magnetic field. In order to design an ideal magnet assembly the magnetocaloric materials and the refrigeration process itself and their properties and performance as a function of magnetic field are investigated. For the magnetocaloric materials it is the magnetization, specific heat capacity and adiabatic temperature that are investigated as functions of the magnetic field. Following this the process utilized by a magnetic refrigerator to provide cooling is investigated using a publicly available one dimensional numerical model. This process is called active magnetic regeneration (AMR). The aim is to determine the performance of the AMR as a function of the magnetic field in order to learn the properties of the optimal magnet assembly. The performance of the AMR as a function of the synchronization and width of the magnetic field with respect to the AMR cycle, the ramp rate and maximum value of the magnetic field are
investigated. Other published magnet designs used in magnetic refrigeration devices are also evaluated, using a figure of merit based on the properties of the investigated magnetocaloric materials, to learn the properties of the best magnet designs to date. Following this investigation the Halbach cylinder, which is a hollow permanent magnet cylinder with a rotating remanent flux density, is investigated in detail as it forms the basis of many magnet designs used in magnetic refrigeration. Here the optimal dimensions of a Halbach cylinder, as well as analytical calculations of the magnetic field for a Halbach cylinder of infinite length, are presented. Once it has been determined which properties are desirable for a magnet used in magnetic refrigeration the design of a new magnet is described. This is a high performance cylindrical magnet for use in a new magnetic refrigeration device being built at Risø DTU. This magnet design must have alternating regions of high and low magnetic field. As a basis for the magnet design the concentric Halbach cylinder design is chosen. This design is then optimized by employing several developed optimization schemes that lower the flux density in a specific region and lower the amount of magnet material used in a given magnet assembly. These schemes are applied to a numerical model of the magnet design. Afterwards the magnet design is dimensioned and segmented to allow construction. This design has been constructed and the flux density measured. Finally, the magnetic forces internally in the magnet design and on the magnetocaloric material inside the magnet assembly have been analyzed.

General information
State: Published
Contributors: Bjørk, R., Bahl, C. R. H., Pryds, N., Smith, A.
Number of pages: 360
Publication date: Sep 2010

Publication information
Place of publication: Roskilde
Publisher: Technical University of Denmark (DTU)
ISBN (Print): 978-87-550-3806-6
Original language: English
Keywords: Magnetic refrigeration, Fuel Cells and Hydrogen, Risø-PhD-57(EN), Risø-PhD-57, Risø-PhD-0057
Electronic versions: Designing_a_magnet.pdf
Source: orbit
Source-ID: 268380
Research output: Research › Ph.D. thesis – Annual report year: 2010

A comprehensive parameter study of an active magnetic regenerator using a 2D numerical model
A two-dimensional numerical heat transfer model is used to investigate an active magnetic regenerator (AMR) based on parallel plates of magnetocaloric material. A large range of parameter variations are performed to study the optimal AMR. The parameters varied are the plate and channel thicknesses, cycle frequency and fluid movement. These are cast into the non-dimensional units utilization, porosity and number of transfer units (NTU). The cooling capacity vs. temperature span is mapped as a function of these parameters and each configuration is evaluated through the maximum temperature span and exergy. The results show that the optimal AMR should have a utilization in the range 0.2–1 and an NTU higher than 10 and not necessarily more than 30. It is concluded that parallel plate-based regenerators face significant challenges in terms of manufacturability. However, the benefit of parallel plate regenerators is a very low pressure drop, which is needed for high performance.

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State: Published
Pages: 753-764
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: International Journal of Refrigeration
Volume: 33
Issue number: 4
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
An experimental study of passive regenerator geometries

General information
State: Published
Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics
Contributors: Engelbrecht, K., Nielsen, K. K., Pryds, N.
Number of pages: 533
Pages: 305-312
Publication date: 2010

An optimized magnet for magnetic refrigeration
A magnet designed for use in a magnetic refrigeration device is presented. The magnet is designed by applying two general schemes for improving a magnet design to a concentric Halbach cylinder magnet design and dimensioning and segmenting this design in an optimum way followed by the construction of the actual magnet. The final design generates a peak value of 1.24 T, an average flux density of 0.9 T in a volume of 2 L using only 7.3 L of magnet, and has an average low flux density of 0.08 T also in a 2 L volume. The working point of all the permanent magnet blocks in the design is very close to the maximum energy density. The final design is characterized in terms of a performance parameter, and it is shown that it is one of the best performing magnet designs published for magnetic refrigeration.

General information
State: Published
Contributors: Bjørk, R., Bahl, C. R. H., Smith, A., Christensen, D., Pryds, N.
Pages: 3324-3328
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 322
Issue number: 21
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.97 SJR 0.786 SNIP 1.349
Web of Science (2017): Impact factor 3.046
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Impact factor 2.63
Web of Science (2016): Indexed yes
Cathode-Electrolyte Interfaces with CGO Barrier Layers in SOFC

Electro microscopy characterization across the cathode–electrolyte interface of two different types of intermediate temperature solid oxide fuel cells (IT-SOFC) is performed to understand the origin of the cell performance disparity. One IT-SOFC cell had a sprayed-cosintered Ce0.90Gd0.01O1.95 (CGO10) barrier layer, the other had a barrier layer deposited by pulsed laser deposition (PLD) CGO10. Scanning electron microscopy, transmission electron microscopy (TEM), and electron backscattered diffraction (EBSD) investigations conclude that the major source of the cell performance difference is attributed to CGO–YSZ interdiffusion in the sprayed-cosintered barrier layer. From TEM and EBSD work, a dense CGO10 PLD layer is found to be deposited epitaxially on the 8YSZ electrolyte substrate—permitting a small amount of SrZrO3 formation and minimizing CGO–YSZ interdiffusion.
Comparison of adjustable permanent magnetic field sources

A permanent magnet assembly in which the flux density can be altered by a mechanical operation is often significantly smaller than comparable electromagnets and also requires no electrical power to operate. In this paper five permanent magnet designs in which the magnetic flux density can be altered are analyzed using numerical simulations, and compared based on the generated magnetic flux density in a sample volume and the amount of magnet material used. The designs are the concentric Halbach cylinder, the two half Halbach cylinders, the two linear Halbach arrays and the four and six rod mangle. The concentric Halbach cylinder design is found to be the best performing design, i.e. the design that provides the most magnetic flux density using the least amount of magnet material. A concentric Halbach cylinder has been constructed and the magnetic flux density, the homogeneity and the direction of the magnetic field are measured and compared with numerical simulation and a good agreement is found.

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Contributors: Bjørk, R., Bahl, C. R. H., Smith, A., Pryds, N.
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Journal: Journal of Magnetism and Magnetic Materials
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Issue number: 22
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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 2.97 SJR 0.786 SNIP 1.349
Web of Science (2017): Impact factor 3.046
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Impact factor 2.63
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.33 SJR 0.73 SNIP 1.296
Web of Science (2015): Impact factor 2.357
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.07 SJR 0.815 SNIP 1.423
Web of Science (2014): Impact factor 1.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.03 SJR 0.801 SNIP 1.385
Web of Science (2013): Impact factor 2.002
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.95 SJR 0.928 SNIP 1.294
Web of Science (2012): Impact factor 1.826
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.84 SJR 1.07 SNIP 1.275
Web of Science (2011): Impact factor 1.78
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.936 SNIP 0.987
Web of Science (2010): Impact factor 1.69
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.844 SNIP 0.908
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.867 SNIP 0.903
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.711 SNIP 0.844
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.838 SNIP 0.882
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.699 SNIP 0.692
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.811 SNIP 1.044
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.051 SNIP 0.957
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.233 SNIP 1.143
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.209 SNIP 0.978
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.832 SNIP 0.936
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.875 SNIP 0.912
Original language: English
Keywords: Magnetic refrigeration, Fuel Cells and Hydrogen
Electronic versions:
Comparison_of_adjustablePermanent_magnetic_field_sources.pdf
Concentration-dependent ionic conductivity and thermal stability of magnetron-sputtered nanocrystalline scandia-stabilized zirconia

Nanocrystalline (nc) scandia-stabilized zirconia (SSZ) electrolytes with scandia contents of 5.9 to 15.9 mol% were synthesized by reactive magnetron sputtering. For scandia content ≥ 9.1 mol%, the as-deposited films were pure cubic phase with <111> texture, while traces of tetragonal phase was found for lower Sc content. Single-line profile analysis of the 111 X-ray diffraction peak yielded an out-of-plane grain size of 10 nm and a microstrain of 2.0-2.2%, regardless of scandia content, for films deposited at 400 °C and a bias of -70 V. Films deposited at higher bias voltages showed a reduced grain size, yielding a grain size of 6 nm and a microstrain of 2.5% at -200 V and -250 V with additional incorporation of argon. Temperature-dependent impedance spectroscopy of the SSZ films showed that the in-plane ionic conductivity had a maximum close to 10.7 mol% and decreased almost an order of magnitude as the scandia - content was increased to 15.9 mol%. The activation energy for oxygen ion migration was determined to be between 1.30 - 1.43 eV. In addition, no dependence on grain size was observed. The above observations suggest a bulk mechanism for ionic conduction.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Electroceramics, Aarhus University, Linköping University
Contributors: Sillassen, M., Eklund, P., Pryds, N., Bonanos, N., Bøttiger, J.
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BFI (2017): BFI-level 1
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Web of Science (2017): Impact factor 2.751
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Impact factor 2.354
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.5 SJR 0.802 SNIP 1.016
Web of Science (2015): Impact factor 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.62 SJR 0.837 SNIP 1.282
Web of Science (2014): Impact factor 2.561
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.35 SJR 0.903 SNIP 1.269
Web of Science (2013): Impact factor 2.112
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Design Concepts for a Continuously Rotating Active Magnetic Regenerator

Design considerations for a prototype magnetic refrigeration device with a continuously rotating AMR are presented. Building the AMR from stacks of elongated plates of the perovskite oxide material La0.67Ca0.33-xSrxMn1.05O3, gives both a low pressure drop and allows grading of the Curie temperature along the plates. This may be accomplished by a novel technique where a compositionally graded material may be tape cast in one piece. The magnet assembly is based on a novel design strategy, to create alternating high- and low magnetic field regions within a magnet assembly. Focus is on maximising the magnetic field in the high field regions but also, importantly, minimising the flux in the low field regions. The design is iteratively optimised through 3D finite element magnetostatic modelling.

General information
State: Published
Effects of dopant concentration and impurities on the conductivity of magnetron-sputtered nanocrystalline yttria-stabilized zirconia

Cubic yttria-stabilized zirconia (YSZ) films with yttria concentrations of 8.7, 9.9, and 11 mol% have been deposited by reactive pulsed DC magnetron from Zr–Y alloy targets. The overall microstructure and texture in the films showed no dependence on the yttria concentration. Films deposited at floating potential had a <111> texture. Single-line profile analysis of the 111 X-ray diffraction peak yielded a grain size of 18 nm and a microstrain of 2%, regardless of deposition temperature. Films deposited at 400 °C and selected bias voltages in the range from − 70 V to − 200 V showed a reduced grain size for higher bias voltages, yielding a grain size of 7 nm and a microstrain of 2.5% at a bias voltage of − 200 V with additional incorporation of argon. Furthermore, the effect of impurities on the ionic conductivity has been investigated, since Hf impurities were found in the samples with yttria concentrations of 8.7, and 9.9 mol%. Temperature-dependent impedance spectroscopy of the YSZ films, deposited at 400 °C and floating potential, showed no variation of the in-plane ionic conductivity with yttria concentration. However, for films deposited at 400 °C and a bias − 70 V, the in-plane ionic conductivity decreased systematically for samples with yttria concentrations of 8.7 and 9.9 mol% compared to the sample with 11 mol% yttria. This suggests that ionic conduction is not a purely bulk mechanism, but mainly related to the grain boundaries. The activation energy for oxygen ion migration was determined to be between 1.25 and 1.32 eV.
Electrical characterization of gadolinia doped ceria films grown by pulsed laser deposition

Electrical characterization of 10 mol% gadolinia doped ceria (CGO10) films of different thicknesses prepared on MgO(100) substrates by pulsed laser deposition is presented. Dense, polycrystalline and textured films characterized by fine grains.
(grain sizes <18 nm and <64 nm for a 20-nm and a 435-nm film, respectively) are obtained in the deposition process. Grain growth is observed under thermal cycling between 300 and 800°C, as indicated by X-ray-based grain-size analysis. However, the conductivity is insensitive to this microstructural evolution but is found to be dependent on the sample thickness. The conductivity of the nanocrystalline films is lower (7.0×10−4 S/cm for the 20-nm film and 3.6×10−3 S/cm for the 435-nm film, both at 500°C) than that of microcrystalline, bulk samples (S/cm at 500°C). The activation energy for the conduction is found to be 0.83 eV for the bulk material, while values of 1.06 and 0.80 eV are obtained for the 20-nm film and the 435-nm film, respectively. The study shows that the ionic conductivity prevails in a broad range of oxygen partial pressures, for example down to about 10−26 atm at 500°C.

**General information**

State: Published
Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics, Microstructures and Interfaces, Ceramic processing, Fuel Cells and Solid State Chemistry Division. Management, Optical Microsensors and Micromaterials, Department of Photonics Engineering
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  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 1
  - Scopus rating (2017): CiteScore 1.62 SJR 0.481 SNIP 0.699
  - Web of Science (2017): Impact factor 1.604
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 1.52 SJR 0.508 SNIP 0.744
  - Web of Science (2016): Impact factor 1.455
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): CiteScore 1.38 SJR 0.519 SNIP 0.768
  - Web of Science (2015): Impact factor 1.444
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): CiteScore 1.74 SJR 0.62 SNIP 0.965
  - Web of Science (2014): Impact factor 1.704
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): CiteScore 1.75 SJR 0.732 SNIP 1.01
  - Web of Science (2013): Impact factor 1.694
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): CiteScore 1.71 SJR 0.843 SNIP 1.033
  - Web of Science (2012): Impact factor 1.545
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): CiteScore 1.77 SJR 0.871 SNIP 1.119
  - Web of Science (2011): Impact factor 1.63
  - ISI indexed (2011): ISI indexed yes
Enhanced conductivity in pulsed laser deposited Ce$_{0.9}$Gd$_{0.1}$O$_{2−\delta}$/SrTiO$_3$ heterostructures

Significant enhancement in the electrical conductivity of Ce$_{0.9}$Gd$_{0.1}$O$_{2−\delta}$ (CGO) thin films (250 and 500 nm) deposited on MgO(001) substrate is observed by introducing ~50 nm thin SrTiO$_3$ buffer layer film. Introduction of the buffer layer is found to form epitaxial films, leading to minimal grain boundary network that results in a free conduction path with near-zero blocking effects perpendicular to current flow. The in-plane conductivity measurements confirm increase in conductivity with increase in compressive strain on CGO films. © 2010 American Institute of Physics
Web of Science (2017): Impact factor 3.495
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Impact factor 3.411
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.47 SJR 1.499 SNIP 1.226
Web of Science (2015): Impact factor 3.142
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.25 SJR 1.861 SNIP 1.492
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.77 SJR 2.146 SNIP 1.633
Web of Science (2013): Impact factor 3.515
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.76 SJR 2.57 SNIP 1.739
Web of Science (2012): Impact factor 3.794
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.04 SJR 2.814 SNIP 1.917
Web of Science (2011): Impact factor 3.844
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Impact factor 3.841
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.012 SNIP 1.916
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.755 SNIP 2.353
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.992 SNIP 2.367
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.897 SNIP 2.275
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 4.018 SNIP 2.414
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 4.281 SNIP 2.22
Web of Science (2001): Indexed yes
Epitaxial growth of atomically flat gadolinia-doped ceria thin films by pulsed laser deposition

Ceria-based thin films are often applied as key functional components in miniaturized electroceramic devices such as solid oxide fuel cells or gas sensors. Processing routes that prevent thermal degradation and yield access to the optimum microstructures are sought. Multi-step growth, involving the preparation of ultrathin seed layers in the first stage of the deposition process is often envisaged to control the growth and physical properties of the subsequent coating. This work suggests that the limitations of conventional pulsed laser deposition (PLD), performed at moderate temperature (400°C), to the growth of dense, gas impermeable 10 mol% gadolinia-doped ceria (CGO10) solid electrolyte can be overcome by the seeding process. In order to evaluate the seed layer preparation, the effects of different thermal annealing treatments on the morphology, microstructure and surface roughness of ultrathin CGO10 layers with a thickness of 4 nm, 13 nm and 22 nm, respectively, grown on Mg(100), were studied by atomic force microscopy and X-ray reflectometry.

Factors controlling the microstructure of Ce0.9Gd0.1O2-δ films in pulsed laser deposition process

Films of Ce0.9Gd0.1O2-δ (CGO10) are prepared at a range of conditions by pulsed laser deposition (PLD) on a single crystal Si (100) and MgO (100), and on a polycrystalline Pt/MgO (100) substrate. The relationship between the film microstructure, crystallography, chemical composition and PLD processing parameters is studied. It is found that the laser fluence has no significant impact on the film density, whereas the substrate temperature and the oxygen pressure are of essential importance for the film microstructure development. The reduction of deposition temperature, down to 250 °C, together with a lowered oxygen pressure of 0.05 mbar, significantly inhibits the growth of columnar structures. Further decrease in oxygen pressure, to 0.005 mbar, promotes films densification, but a stress build-up is observed and leads to a lattice-parameter enlargement of the coatings. The chemical films composition is affected by the applied fluence. At a low fluence, 0.5 J/cm², a congruent transfer is obtained while a relative Gd enrichment results for substantially higher (3.5-5.5 J/cm²).
High Temperature Thermoelectric Ceramic Materials

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Xu, J. J., Van Nong, N., Yanangiya, S., Sonne, M., Pryds, N.
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Publisher: Dansk Metallurgisk Selskab
Editor: Brandsted, P.
ISBN (Print): 87-87535-40-8
Keywords: Magnetic refrigeration, Fuel Cells and hydrogen
Source: orbit
Source-ID: 258084
Research output: Research › Article in proceedings – Annual report year: 2010

High Temperature Thermoelectric Performance of Nano-scale Misfit-layered Ca3Co4O9 with Ga Substitution

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Kyushu University
Contributors: Van Nong, N., Xu, J. J., Yanagiya, S., Pryds, N., Ohtaki, M.
Publication date: 2010

Host publication information
Title of host publication: Abstract book
Keywords: Magnetic refrigeration
Electronic versions: Van Nong abstract.pdf
Source: orbit
Source-ID: 275379
Research output: Research › Conference abstract in proceedings – Annual report year: 2011

High thermoelectric performance of reduced lanthanide molybdenum oxides densified by spark plasma sintering

Four highly reduced molybdenum oxides LnMo8O14 (Ln = La, Ce, Nd and Sm) containing bicapped Mo8 clusters were synthesized via solid state reaction followed by spark plasma sintering. The thermoelectric properties were investigated, and NdMo8O14 exhibits the best performance with the maximum power factor of 177 μW.mK² at 1000 K. The highest ZT of NdMo8O14 was determined to be around 0.1 at 1000 K.

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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Stockholm University, University of Waterloo
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Journal: Journal of Alloys and Compounds
Volume: 500
Improvement of Niobium Doped SrTiO3 by Nanostructuring

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Contributors: Sonne, M., Van Nong, N., He, Z., Pryds, N., Linderoth, S.
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Sonne_paper.pdf
Source: orbit
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2011

Interfacial properties of immiscible Co-Cu alloys
Using electromagnetic levitation under microgravity conditions, the interfacial properties of an Cu75Co25 alloy have been investigated in the liquid phase. This alloy exhibits a metastable liquid miscibility gap and can be prepared and levitated in a configuration consisting of a liquid cobalt-rich core surrounded by a liquid copper-rich shell. Exciting drop oscillations and analysing the frequency spectrum, both surface and (liquid–liquid) interfacial tension can be derived from the observed oscillation frequencies. This paper briefly reviews the theoretical background and reports on a recent experiment carried out on board the TEXUS 44 sounding rocket.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, German Aerospace Center, Centre Interdisciplinaire de Nanosciences de Marseille, University of Turin, University of Copenhagen
Contributors: Egry, I., Ratke, L., Kolbe, M., Chatain, D., Curiotto, S., Battezzati, L., Johnson, E., Pryds, N.
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Journal: Journal of Materials Science
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Investigation of table-like entropy change around room temperature in La0.75Ca0.25-xSrxMnO3 manganites

General information
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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Electrocermics
Contributors: Krishnan Venkatesh, R., Pryds, N., Kuhn, L. T.
Publication date: 2010

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Title of host publication: Proceedings
Publisher: International Institute of Refrigeration
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2010

Low-Temperature Superionic Conductivity in Strained Yttria-Stabilized Zirconia

Very high lateral ionic conductivities in epitaxial cubic yttria-stabilized zirconia (YSZ) synthesized on single-crystal SrTiO3 and MgO substrates by reactive direct current magnetron sputtering are reported. Superionic conductivities (i.e., ionic conductivities of the order 10^-1 cm^-1) are observed at 500 °C for 58-nm-thick films on MgO. The results indicate a superposition of two parallel contributions - one due to bulk conductivity and one attributable to conduction along the film-substrate interface. Interfacial effects dominate the conductivity at low temperatures.

General information
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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division, Aarhus University, Linköping University
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Web of Science (2017): Impact factor 13.325
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Impact factor 12.124
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Modeling of parallel-plate regenerators with non-uniform plate distributions

A two-dimensional finite element model describing the performance of parallel-plate regenerators with arbitrary channel width distributions has been developed in order to investigate the effect of non-uniform plate spacing on the performance of regenerators. Results for a series of hypothetical plate spacing distributions are presented in order to understand the impact of spacing non-uniformity. Simulations of more realistic distributions where the plate spacings follow normal distributions are then discussed in order to describe the deviation of the performance of a regenerator relative to one with uniform spacing as a function of the standard deviation of the plate distribution. It has been shown that the most significant reduction in performance occurs when a volume of fluid between 100% and 200% of the regenerator void volume is displaced in a single blow.

General information
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Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics, Thermal Energy, Department of Mechanical Engineering, University of Wisconsin-Madison
Pages: 5065-5072
Publication date: 2010
Peer-reviewed: Yes

Publication information
Volume: 53
Numerical modeling and analysis of the active magnetic regenerator

In this thesis the active magnetic regenerator (AMR) is analyzed using various numerical tools and experimental devices. A 2-dimensional transient numerical model of the AMR is developed and implemented and it is used to investigate the influence of a range of parameters on the performance of the AMR. The model simulates a regenerator made of parallel plates. The operating parameters, such as airflow rates, thermal utilization, magnetocaloric properties etc. are varied as are geometric properties such as plate and channel thickness, regenerator length and porosity. In this way the performance expressed as temperature span versus cooling power is mapped as a function of the central parameters.

Since regenerators built of several magnetic materials distinguished by their respective magnetic transition temperatures are reported to perform better than single-material AMRs this concept has been investigated using the numerical AMR model. The results show indeed that the performance may be enhanced significantly and it may thus be concluded that the performance of the AMR is dependent on a vast number of parameters (material composition, magnetic field source, regenerator geometry, regenerator efficiency, operating conditions etc.). The results presented in this thesis thus provide an overview of the influence of many of these parameters on the AMR performance. It is also concluded that the internal field of an AMR is far from homogeneous. Indeed, it does depend on both regenerator geometry, orientation of the applied field, the temperature distribution in the material and the material composition. A magnetostatic 3-dimensional model is developed (by the author of this thesis in close collaboration with Mr. D.V. Christensen, Ris DTU). The results from this show that the resulting internal field in an active regenerator may vary so significantly that clearly preferable configurations exist and in particular that certain configurations should not be considered. The combination of the model for the internal field and the transient AMR model has not been fully implemented and the performance impact of the internal field model remains thus to be investigated. Finally, suggestions for future work are provided based on the knowledge presented here. These include alternative regenerator geometries, a list of physical effects that have not been investigated in terms of their impact on the AMR performance yet etc. Several ready-to-go projects are thus suggested for future work.

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Research output: Research › Ph.D. thesis – Annual report year: 2010

Numerical modeling of graded active magnetic regenerators

General information
State: Published
Organisations: Manufacturing Engineering, Department of Mechanical Engineering, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
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Processing and Characterization of ZnO-based Thermoelectric Materials

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Contributors: He, Z., Van Nong, N., Sonne, M., Pryds, N., Linderoth, S.
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Electronic versions:
Zeming He_paper.pdf
Source: orbit
Source-ID: 275398
Research output: Research - peer-review › Article in proceedings – Annual report year: 2011

Pulsed laser deposition of gadolinia doped ceria layers at moderate temperature – a seeding approach
Ceria-based thin films are often applied as key functional components in miniaturized electroceramic devices such as solid oxide fuel cells or gas sensors. Processing routes that prevent thermal degradation and yield access to the optimum microstructures are sought. Multi-step growth, involving the preparation of ultrathin seed layers in the first stage of the deposition process is often envisaged to control the growth and physical properties of the subsequent coating. This work suggests that the limitations of conventional pulsed laser deposition (PLD), performed at moderate temperature (400°C), to the growth of dense, gas impermeable 10 mol% gadolinia-doped ceria (CGO10) solid electrolyte can be overcome by the seeding process. In order to evaluate the seed layer preparation, the effects of different thermal annealing treatments on the morphology, microstructure and surface roughness of ultrathin CGO10 layers with a thickness of 4 nm, 13 nm and 22 nm, respectively, grown on Mg(100), were studied by atomic force microscopy and X-ray reflectometry.

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Electronic versions:
bookabstracts_280910_2.pdf
URLs:
Source: orbit
Source-ID: 267609
Research output: Research - peer-review › Poster – Annual report year: 2010

Quantitative TEM analysis of Al/Cu multilayer systems prepared by pulsed laser deposition
Thin films composed of alternating Al/Cu/Al layers were deposited on a (111) Si substrate using pulsed laser deposition (PLD). The thicknesses of the film and the individual layers, and the detailed internal structure within the layers were characterized by means of transmission electron microscopy (TEM), high-resolution TEM (HRTEM), and energy-filtered TEM (EFTEM). Each Al or Cu layer consists of a single layer of nano-sized grains of different orientations. EFTEM results revealed a layer of oxide about 2 nm thick on the surface of the Si substrate, which is considered to be the reason for the formation of the first layer of nano-sized Al grains. The results demonstrate that the PLD technique is a powerful tool to produce nano-scale multilayered metal films with controllable thickness and grain sizes.
Resistance switching at the interface of LaAlO3/SrTiO3

At the interface of LaAlO3/SrTiO3 with film thickness of 3 unit cells or greater, a reproducible electric-field-induced bipolar resistance switching of the interfacial conduction is observed on nanometer scale by a biased conducting atomic force microscopy under vacuum environment. The switching behavior is suggested to be an intrinsic feature of the SrTiO3 single crystal substrates, which mainly originates from the modulation of oxygen ion transfer in SrTiO3 surface by external electric field in the vicinity of interface, whereas the LaAlO3 film acts as a barrier layer. © 2010 American Institute of Physics

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Chinese Academy of Sciences
Contributors: Chen, Y., Zhao, J., Sun, J., Pryds, N., Shen, B.
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Publication date: 2010
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Impact factor 3.495
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Impact factor 3.411
Web of Science (2016): Indexed yes
Review and comparison of magnet designs for magnetic refrigeration

One of the key issues in magnetic refrigeration is generating the magnetic field that the magnetocaloric material must be subjected to. The magnet constitutes a major part of the expense of a complete magnetic refrigeration system and a large effort should therefore be invested in improving the magnet design. A detailed analysis of the efficiency of different published permanent magnet designs used in magnetic refrigeration applications is presented in this paper. Each design is analyzed based on the generated magnetic flux density, the volume of the region where this flux is generated and the amount of magnet material used. This is done by characterizing each design by a figure of merit magnet design efficiency parameter, \( \Lambda_{\text{cool}} \). The designs are then compared and the best design found. Finally recommendations for designing the ideal magnet design are presented based on the analysis of the reviewed designs.

General information

State: Published
Contributors: Bjørk, R., Bahl, C. R. H., Smith, A., Pryds, N.
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Peer-reviewed: Yes

Publication information

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Scopus rating (2017): CiteScore 3.46 SJR 1.471 SNIP 1.888
Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.44 SJR 1.349 SNIP 1.532
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.6 SJR 1.619 SNIP 2.086
Web of Science (2014): Impact factor 2.241
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.25 SJR 1.422 SNIP 1.944
Web of Science (2013): Impact factor 1.702
ISI indexed (2013): ISI indexed yes
Structural and magnetic properties of Gd/Fe multilayers grown by pulsed laser deposition

This work investigates the structural and the magnetic properties of Gd/Fe multilayered thin films grown by pulsed laser deposition onto Si (001) substrates at room temperature. The Fe layer thickness is varied from 70 to 150 nm and its effect on the structural and magnetic properties of Fe/Gd/Fe sandwich multilayers has been explored. Gd films were found to change from amorphous to polycrystalline at a critical thickness of 20 nm.

General information
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Contributors: Kant, K. M., Bahl, C. R. H., Pryds, N., Smith, A., Schou, J.
Pages: 576-579
Publication date: 2010
Peer-reviewed: Yes
The Effect of (Ag, Ni, Zn)-Addition on the Thermoelectric Properties of Copper Aluminate

Polycrystalline bulk copper aluminate Cu1-x-yAgxByAlO2 with B = Ni or Zn were prepared by spark plasma sintering and subsequent thermal treatment. The influence of partial substitution of Ag, Ni and Zn for Cu-sites in CuAlO2 on the high temperature thermoelectric properties has been studied. The addition of Ag and Zn was found to enhance the formation of CuAlO2 phase and to increase the electrical conductivity. The addition of Ag or Ag and Ni on the other hand decreases the electrical conductivity. The highest power factor of $1.26 \times 10^{-4}$ W/mK2 was obtained for the addition of Ag and Zn at 1,060 K, indicating a significant improvement compared with the non-doped CuAlO2 sample.
The persistence of the magnetocaloric effect in (La1-x)A(x)(0.67)Ba0.33Mn1.05O3-δ

Polycrystalline samples of (La1-x)A(x)0.67Ba0.33Mn1.05O3-δ, with A being a mixture of lanthanides containing 66% La, 22% Nd, 8% Pr and 4% Ce, were prepared by the glycine-nitrate method, with target compositions of x = 0, 0.33, 0.67 and 1. The effect of the mixture of lanthanides on the Curie temperature, TC, and the magnetocaloric properties was investigated. The prepared samples are single phase, with space group R-3c. The lattice parameters and average A-site ionic radius, RA decrease linearly with x while the size disorder, as characterized by the variance, σ2, increases from 0.014 to 0.017 with x. As x is increased, the increase in σ2 drives a linear decrease in TC. The magnetic entropy change, ΔSM, for a field change of 1 T is obtained by magnetization measurements, giving a maximum value of 1.7 J/kg K, and a relative cooling power, RCP, of 43 J/kg, independent of x. These results suggest that replacing lanthanum with a mixture of lanthanides is a realistic way to tune the working temperature of magnetocaloric manganites while maintaining a constant magnetocaloric effect.

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Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Physics
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Issue number: 7
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.03 SJR 0.739 SNIP 0.953
Web of Science (2017): Impact factor 2.176
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.72 SJR 0.906 SNIP 0.977
Web of Science (2016): Impact factor 2.068
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.57 SJR 0.821 SNIP 0.996
Web of Science (2015): Impact factor 2.101
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.04 SJR 1.039 SNIP 1.197
Web of Science (2014): Impact factor 2.183
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.24 SJR 1.155 SNIP 1.286
Web of Science (2013): Impact factor 2.185
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.13 SJR 1.312 SNIP 1.291
Web of Science (2012): Impact factor 2.21
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.24 SJR 1.374 SNIP 1.3
Web of Science (2011): Impact factor 2.168
Thermoelectric properties of LnMo8O14 (Ln=La, Pr, Nd and Sm)

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, University of Waterloo, Stockholm University, Clemson University
Contributors: Xu, J. J., Sonne, M., Kleinke, H., Nygren, M., Tritt, T., Pryds, N.
Publication date: 2010

Host publication information
Title of host publication: Proceedings (Ceramic Transactions).
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URLs:
Source: orbit
Source-ID: 249636
Research output: Research › Article in proceedings – Annual report year: 2009
Thermoelectric properties of molybdenum oxides LnMo(8)O(14) (Ln = La, Ce, Pr, Nd and Sm)

The series LnMo8O14 (Ln = La, Ce, Pr, Nd and Sm) containing bicapped Mo8 clusters was synthesized via solid state reaction at 1673 K. Oxides of this type were reported to be narrow gap semiconductors. Our Seebeck coefficient measurements show that some of these reduced molybdenum oxides exhibit a thermopower of above −100 μV/K at room temperature, which is promising for the thermoelectric application. The highest power factor of 71 μW/mK2 was obtained for SmMo8O14 at 1152 K.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, University of Waterloo
Contributors: Xu, J. J., Sonne, M., Pryds, N., Kleinke, H.
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Journal: Journal of Alloys and Compounds
Volume: 489
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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
Web of Science (2015): Impact factor 3.014
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.13 SJR 1.117 SNIP 1.632
Web of Science (2014): Impact factor 2.999
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.73 SJR 1.059 SNIP 1.583
Web of Science (2013): Impact factor 2.726
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.43 SJR 1.246 SNIP 1.57
Web of Science (2012): Impact factor 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.41 SJR 1.164 SNIP 1.463
Web of Science (2011): Impact factor 2.289
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
The solidification in the presence of a metastable miscibility gap: the case of Co-Cu and Co-Cu-X alloys

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, University of Turin
Contributors: Battezzati, L., Johnson, E., Pryds, N., Penna, A., Curiotto, S.
Pages: 41-46
Publication date: 2010
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Publication information
Journal: Materials Science Forum
Volume: 649
ISSN (Print): 0255-5476
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.3 SJR 0.18 SNIP 0.317
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.28 SJR 0.188 SNIP 0.302
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.29 SJR 0.218 SNIP 0.326
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.33 SJR 0.261 SNIP 0.414
Web of Science (2014): Indexed yes
2-dimensional numerical modeling of active magnetic regeneration

Various aspects of numerical modeling of Active Magnetic Regeneration (AMR) are presented. Using a 2-dimensional numerical model for solving the unsteady heat transfer equations for the AMR system, a range of physical effects on both idealized and non-idealized AMR are investigated. The modeled system represents a linear, parallel-plate based AMR. The idealized version of the model is able to predict the theoretical performance of AMR in terms of cooling power and temperature span. This is useful to a certain extent, but a model reproducing experiments to a higher degree is desirable. Therefore physical effects such as thermal parasitic losses have been included. Furthermore, experimentally found magnetocaloric properties are used when available, since the commonly used mean field model can be too idealized and is not always able to determine the magnetocaloric effect accurately. In the present paper preliminary conclusions on which non-ideal physical effects are thought to be dominating considering the performance of experimental AMR are given. The modeling results are compared to experimental results from the AMR test device situated at Risø DTU, Technical University of Denmark. The experimental validation shows that using the measured magnetocaloric properties significantly improves the modeling results compared to using the mean field model.
Crossover of angular dependent magnetoresistance with the metal-insulator transition in colossal magnetostrictive manganite films

The temperature and magnetic field dependence of angular dependent magnetoresistance (AMR) along two orthogonal directions ([100] and [01]) was investigated in a charge-orbital-ordered Sm0.5Ca0.5MnO3 (SCMO) film grown on (011)-oriented SrTiO3 substrates. A dramatic decrease of AMR magnitude in both directions was observed with the appearance of magnetic-field-induced metal-insulator transition, which further led to a sign crossover in the AMR effect. The AMR crossover may give a direct evidence of the drastic modification of electronic structure or possible orbital reconstruction with the magnetic-destruction of charge/orbital ordering in SCMO films. ©2009 American Institute of Physics
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Impact factor 3.495
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Impact factor 3.411
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.47 SJR 1.499 SNIP 1.226
Web of Science (2015): Impact factor 3.142
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.25 SJR 1.861 SNIP 1.492
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.77 SJR 2.146 SNIP 1.633
Web of Science (2013): Impact factor 3.515
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.76 SJR 2.57 SNIP 1.739
Web of Science (2012): Impact factor 3.794
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.04 SJR 2.814 SNIP 1.917
Web of Science (2011): Impact factor 3.844
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Impact factor 3.841
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.012 SNIP 1.916
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.755 SNIP 2.353
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.992 SNIP 2.367
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.897 SNIP 2.275
Detailed numerical modeling of a linear parallel-plate Active Magnetic Regenerator

A numerical model simulating Active Magnetic Regeneration (AMR) is presented and compared to a selection of experiments. The model is an extension and re-implementation of a previous two-dimensional model. The new model is extended to 2.5D, meaning that parasitic thermal losses are included in the spatially not-resolved direction. The implementation of the magnetocaloric effect (MCE) is made possible through a source term in the heat equation for the magnetocaloric material (MCM). This adds the possibility to model a continuously varying magnetic field. The adiabatic temperature change of the used gadolinium has been measured and is used as an alternative MCE than mean field modeling. The results show that using the 2.5D formulation brings the model significantly closer to the experiment. Good agreement between the experimental results and the modeling was obtained when using the 2.5D formulation in combination with the measured adiabatic temperature change.

General information
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Organisations: Department of Mechanical Engineering, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
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Journal: International Journal of Refrigeration
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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 3.46 SJR 1.471 SNIP 1.888
Web of Science (2017): Impact factor 3.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Impact factor 2.779
Web of Science (2016): Indexed yes
Do simple magnetic refrigeration test devices lead to more successful prototypes?

General information
State: Published
Contributors: Pryds, N., Bahl, C. R. H., Smith, A.
Publication date: 2009

Host publication information
Title of host publication: Proceedings
Publisher: Iowa State University
Keywords: Magnetic refrigeration, Fuel Cells and hydrogen
Source: orbit
Source-ID: 243963
Research output: Research - peer-review › Article in proceedings – Annual report year: 2009

Experiments on a Modular Magnetic Refrigeration Device

General information
State: Published
Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Rise National Laboratory for Sustainable Energy, Thermo Ceramics
Contributors: Engelbrecht, K., Jensen, J. B., Bahl, C. R. H., Pryds, N.
Pages: 431-436
Publication date: 2009

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Place of publication: Paris
Publisher: Institut International du Froid
ISBN (Print): 978-2-913149-67-0
(Science et Technique du Froid, Comptes Rendus; No. 2009-3).
Keywords: Magnetic refrigeration, Fuel Cells and hydrogen
Source: orbit
Source-ID: 253896
Research output: Research - peer-review › Article in proceedings – Annual report year: 2009

Factors controlling the microstructure of Ce0.9Gd0.1O2-δ films in pulsed laser deposition process

Films of Ce0.9Gd0.1O2-δ(CGO10) are prepared at a range of conditions by pulsed laser deposition (PLD) on a single crystal Si (100) and MgO (100), and on a polycrystalline Pt/MgO (100) substrate. The relationship between the film microstructure, crystallography, chemical composition and PLD processing parameters is studied. It is found that the laser fluence has no significant impact on the film density, whereas the substrate temperature and the oxygen pressure are of essential importance for the film microstructure development. The reduction of deposition temperature down to 250 oC together with a lowered oxygen pressure of 0.05 mbar, significantly inhibits the growth of columnar structures. Further decrease in oxygen pressure, to 0.005 mbar, promotes film densifications, but a stress build-up is observed and leads to a lattice-parameter enlargement of the coatings. The chemical films composition is affected by the applied fluence. At a low fluence, 0.5 J/cm², a congruent transfer is obtained while a relative Gd enrichment results for substantially higher fluences (3.5-5.5 J/cm²).

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Keywords: gadolinia-doped ceria, stress, low temperature deposition, pulsed laser deposition
URLs:
Giant magnetoresistance in melt spun Cu85Co10Ni5
CuCoNi rapidly solidified alloys are interesting because they display giant magnetoresistance (GMR). In the present work a Cu85Co10Ni5 alloy has been synthesized by melt spinning and analysed for GMR. The ribbons obtained have been annealed at different temperatures and the evolution of the crystal structure with annealing has been studied by X-ray diffraction. The microstructure has been observed by TEM and related to the magnetic properties, investigated in a vibrating sample magnetometer. In the studied composition the magnetoresistance was found to be lower than in binary CuCo alloys without Ni addition. (C) 2008 Elsevier B.V. All rights reserved.
Ionic conductivity and thermal stability of magnetron-sputtered nanocrystalline yttria-stabilized zirconia

Thermally stable, stoichiometric, cubic yttria-stabilized zirconia (YSZ) thin-film electrolytes have been synthesized by reactive pulsed dc magnetron sputtering from a Zr–Y (80/20 at. %) alloy target. Films deposited at floating potential had a texture. Single-line profile analysis of the 111 x-ray diffraction peak yielded a grain size of ~20 nm and a microstrain of ~2% regardless of deposition temperature. Films deposited at 400 °C and selected bias voltages in the range from −70 to −200 V showed a reduced grain size for higher bias voltages, yielding a grain size of ~6 nm and a microstrain of ~2.5% at bias voltages of −175 and −200 V with additional incorporation of argon. The films were thermally stable; very limited grain coarsening was observed up to an annealing temperature of 800 °C. Temperature-dependent impedance spectroscopy analysis of the YSZ films with Ag electrodes showed that the in-plane ionic conductivity was within one order of magnitude higher in films deposited with substrate bias corresponding to a decrease in grain size compared to films deposited at floating potential. This suggests that there is a significant contribution to the ionic conductivity from grain boundaries. The activation energy for oxygen ion migration was determined to be between 1.14 and 1.30 eV. ©2009 American Institute of Physics
Large anisotropy in colossal magnetoresistance of charge orbital ordered epitaxial Sm0.5Ca0.5MnO3 films

We investigated the structure and magnetotransport properties of Sm0.5Ca0.5MnO3 (SCMO) films epitaxially grown on (011)-oriented SrTiO3 substrates, which exhibited clear charge/orbital ordering transition. A significant anisotropy of ~1000 in the colossal magnetoresistance (CMR) effect was observed in the films with a thickness between 50 and 80 nm, which was distinctly different from the basically isotropic CMR effect in bulk SCMO. The large anisotropy in the CMR can be ascribed to the intrinsic asymmetric strain in the film, which plays an important role in tuning the spin–orbit coupling in manganite films. The origin of the peculiar CMR effect is discussed.

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Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Chinese Academy of Sciences
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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 2.37 SJR 0.875 SNIP 0.921
Web of Science (2017): Impact factor 2.617
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.89 SJR 1.553 SNIP 0.91
Web of Science (2016): Impact factor 2.678
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.65 SJR 1.043 SNIP 0.889
Web of Science (2015): Impact factor 2.209
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.99 SJR 1.284 SNIP 0.987
Web of Science (2014): Impact factor 2.346
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.11 SJR 1.326 SNIP 1.022
Web of Science (2013): Impact factor 2.223
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.33 SJR 1.688 SNIP 1.168
Web of Science (2012): Impact factor 2.355
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.31 SJR 1.66 SNIP 1.161
Web of Science (2011): Impact factor 2.546
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.663 SNIP 1.054
Web of Science (2010): Impact factor 2.332
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.525 SNIP 1.015
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.467 SNIP 1.071
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.561 SNIP 1.143
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.689 SNIP 1.229
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.725 SNIP 1.174
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.587 SNIP 1.19
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.464 SNIP 1.06
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.364 SNIP 1.223
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.376 SNIP 1.045
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.411 SNIP 1.093
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.384 SNIP 1.124

Original language: English
Magnetic cooling at Risø DTU
Magnetic refrigeration at room temperature is of great interest due to a long-term goal of making refrigeration more energy-efficient, less noisy and free of any environmentally hostile materials. A refrigerator utilizing an active magnetic regenerator (AMR) is based on the magnetocaloric effect, which manifests itself as a temperature change in magnetic materials when subjected to a varying magnetic field. In this work we present the current state of magnetic refrigeration research at Risø DTU with emphasis on the numerical modeling of an existing AMR test machine. A 2D numerical heat-transfer and fluid-flow model that represents the experimental setup is presented. Experimental data of both no-heat load and heat load situations are compared to the model. Moreover, results from the numerical modeling of the permanent magnet design used in the system are presented.

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DOIs:
10.1016/j.scriptamat.2012.08.036
URLs:
http://arxiv.org/abs/0902.0812v1
Source: orbit
Source-ID: 239394
Research output: Research › Journal article – Annual report year: 2009

Magnetic Refrigeration – an Energy Efficient Technology for the Future
Magnetic refrigeration is an emerging technology that has the potential to significantly reduce the energy consumption in the refrigeration sector. The technology relies on the heating and cooling of magnetic materials upon the application and removal of a magnetic field, respectively. This magnetocaloric effect is inherent to all magnetic materials, but manifests itself stronger in some materials. The thermodynamically reversible nature of the magnetocaloric effect holds out the promise of a more energy efficient method of refrigeration compared to conventional compressor technology. Coupling this with an absence of ozone depleting and greenhouse contributing gasses gives magnetic refrigeration the potential to become an environmentally sustainable technology. The magnetic refrigeration group at Risø DTU aims to demonstrate the technology in a prototype magnetic refrigeration device. Our work spans a wide range of scientific and technological areas. At the pure science end there is the development and understanding of new magnetocaloric materials, while the design and implementation of a prototype device along with the processing of materials is at the technological engineering end. Tying the work together are advanced numerical computer models of the individual parts of the prototype. A simple yet versatile test machine located at Risø DTU is used to test and characterise new materials and to test the design, configuration and operating conditions relevant for a prototype device, while ensuring understanding through consistency with the numerical models.

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State: Published
Number of pages: 316
Pages: 107-115
Magnetocaloric effect in (La1-xAx)2/3Ba1/3Mn1.05O3-δ

Recently, a large magnetocaloric effect has been reported in La2/3Ba1/3MnO3-δ at about 300 K. In this paper, we investigate the effect of the ion size distribution at the A site on the magnetocaloric effect of this perovskite material. This is accomplished by replacing the lanthanum by Ce, Pr, and Nd, which allows us to study the effect of both the average size, , and the distribution, σrA, on the magnetic properties of the system. Using magnetization and heat capacity measurements, we determine the important magnetocaloric parameters ΔSM and ΔTad of (La1-xAx)2/3Ba1/3Mn1.05O3-δ powders prepared by the Glycine-Nitrate method.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Ancona-Torres, C. E., Menon, M., Bahl, C. R. H., Pryds, N., Linderoth, S.
Publication date: 2009
Peer-reviewed: No
Event: Poster session presented at European Congress on Advanced Materials and Processes 2009, Glasgow, United Kingdom.
Keywords: Ceramic processing, Fuel Cells and Solid State Chemistry Division. Management
Source: orbit
Source-ID: 266199
Research output: Research › Poster – Annual report year: 2009

Numerical modeling in magnetic refrigeration

General information
State: Published
Publication date: 2009

Host publication information
Numerical Modeling of Multi-Material Active Magnetic Regeneration

Magnetic refrigeration is a potentially environmentally-friendly alternative to vapour compression technology that is presented in this paper. The magnetocaloric effect in two magnetocaloric compounds in the La(Fe,Co,Si)13 series is presented in terms of their adiabatic temperature change and the specific heat as a function of temperature at constant magnetic field. A 2.5-dimensional numerical model of an active magnetic regenerative (AMR) refrigerator device is presented. The experimental AMR located at Risø DTU has been equipped with a parallel-plate based regenerator made of the two materials. Experimental zero heat-load temperature spans are presented for different operating conditions and the results are compared to predictions of the numerical model. It is concluded that the model reproduces the experimental tendencies and when including thermal parasitic losses to ambient and the predictions from the model are within 1.5 K of the experimental results.

On the growth of gadolinia-doped ceria by pulsed laser deposition

In order to establish a new platform to manufacture micro sized solid oxide fuel cells (SOFCs) with low operating temperatures, new design concepts, new preparation methods and new materials are being explored. Our studies in this paper are focused on the electrolyte material, and in particular gadolinia doped ceria (GDC), an electrolytematerial, likely to replace the traditional yttria-stabilised zirconia (YSZ) for low temperature applications. GDC films were grown on a single crystal Si by pulsed laser deposition (PLD). The microstructure of the films as a function of growth time has been studied. We have found that the mean grain size increases with film thickness h as h^{2/5}, in agreement with theoretical results.
On the optimal magnet design for magnetic refrigeration

General information
State: Published
Contributors: Bjørk, R., Bahl, C. R. H., Smith, A., Pryds, N.
Publication date: 2009

Host publication information
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Publisher: Institut International du Froid
ISBN (Print): 978-2-913149-67-0
(Science et Technique du Froid, Comptes Rendus; No. 2009-3).
Keywords: Magnetic refrigeration, Fuel Cells and hydrogen
Source: orbit
Source-ID: 253895
Research output: Research - peer-review › Article in proceedings – Annual report year: 2009

Quantitative TEM analysis of Al/Cu multilayer prepared by pulsed laser deposition

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Optical Microsensors and Micromaterials, Department of Photonics Engineering
Contributors: Liu, H., Pryds, N., Schou, J., Huang, X.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 10th International Conference on Laser Ablation, Singapore, Singapore.
Keywords: Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 254086
Research output: Research - peer-review › Poster – Annual report year: 2009

RHEED study of titanium dioxide with pulsed laser deposition
Reflection high-energy electron diffraction (RHEED) operated at high pressure has been used to monitor the growth of thin films of titanium dioxide (TiO2) on (1 0 0) magnesium oxide (MgO) substrates by pulsed laser deposition (PLD). The deposition is performed with a synthetic rutile TiO2 target at low fluence. The topography and structure of the deposited layers are characterized using in situ high pressure RHEED and atomic force microscope (AFM). Based on these observations the growth mode of the films is discussed. The results will be compared to earlier results obtained for the growth of TiN films on (1 0 0) MgO

General information
The effect of impurity doping for thermoelectric properties of CuAlO2

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Hakodate National College of Technology
Contributors: Yanagiya, S., Xu, J. J., Pryds, N.
Publication date: 2009
Peer-reviewed: No
Keywords: Solid Oxide Fuel Cells, Fuel Cells and hydrogen
Source: orbit
Source-ID: 248728
Research output: Research › Poster – Annual report year: 2009
The effect of manganese stoichiometry on the Curie temperature of La0.67Ca0.26Sr0.07Mn1+XO3 used in magnetic refrigeration

General information
State: Published
Organisations: Ceramic processing, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics
Contributors: Biering, I., Menon, M., Pryds, N.
Pages: 71-76
Publication date: 2009

Host publication information
Title of host publication: Advances in Energy Materials
Volume: 205
Publisher: American Ceramic Society
ISBN (Print): 978-0-470-40843-8
Keywords: Magnetic refrigeration
Source: orbit
Source-ID: 276048
Research output: Research - peer-review › Article in proceedings – Annual report year: 2009

Thermoelectric properties of LnMo8O14 (Ln = La, Pr, Nd, and Sm)

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Xu, J. J., Sonne, M., Kleinke, H., Nygren, M., Tritt, T., Pryds, N.
Publication date: 2009
Peer-reviewed: No
Event: Poster session presented at The 28th International Conference on Thermoelectrics and the 7th European Conference on Thermoelectrics, Freiburg (DE), 26-30 July, .
Keywords: Solid Oxide Fuel Cells, Fuel Cells and hydrogen
Source: orbit
Source-ID: 248729
Research output: Research › Poster – Annual report year: 2009

Transport properties of nanocrystalline gadolinia doped ceria films grown by pulsed laser deposition

General information
State: Published
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 10th International Conference on Laser Ablation, Singapore, Singapore.
Keywords: Solid Oxide Fuel Cells, Fuel Cells and hydrogen
Source: orbit
Source-ID: 254084
Research output: Research - peer-review › Poster – Annual report year: 2009

Numerical modelling and analysis of a room temperature magnetic refrigeration system
This thesis presents a two-dimensional mathematical model of an Active Magnetic Regenerator (AMR) system which is used for magnetic refrigeration at room temperature. The purpose of the model is to simulate a laboratory-scale AMR constructed at Risø National Laboratory. The AMR model geometry comprises a regenerator made of parallel plates, which are separated by channels of a heat transfer fluid. The time-dependent model solves the momentum and continuity equations of the flow of the heat transfer fluid and the coupled energy equations of the heat transfer in the regenerator and the fluid. The AMR performs a cyclic process, and to simulate the AMR refrigeration cycle the model starts from an initial temperature distribution in the regenerator and fluid channel and takes time steps forward in time until the cyclical steady-state is obtained. The model can therefore be used to study both transient and steady-state phenomena. The AMR
performance can be evaluated in terms of the no-load temperature span as well as the refrigeration capacity and the COP. The AMR model was verified extensively and it was concluded that the model has energy conservation and that the solution is independent of the chosen grid and time step. Initial results from the model showed significant temperature differences in both the regenerator and the fluid channel during the AMR cycle. This justifies the use of two-dimensional methods when an AMR with a parallel-plate regenerator is modelled. The model is flexible and was used to perform several parametric studies of the AMR performance for different design choices and operating conditions. The results of these studies are presented and the implications for optimal AMR operation are discussed. Finally, the AMR model was validated by comparing the model result to measurements from the experimental AMR constructed by Risø. The validation shows good agreement between the model and the experiments and it is possible to predict both the trends as well as the temperature span of the experimental AMR. In addition, the model can estimate the optimal operating conditions with good accuracy. The ability to provide good results of both the behavior and the performance of the experimental AMR shows that the developed model is a useful tool, which may be used for analysis, design and optimization of the laboratory AMR.

General information
State: Published
Management, Thermal Energy
Contributors: Petersen, T. F., Pryds, N., Smith, A., Linderoth, S., Elmegaard, B., Knudsen, H. H.
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Place of publication: Roskilde
Publisher: Danmarks Tekniske Universitet, Risø Nationallaboratoriet for Bæredygtig Energi
ISBN (Print): 978-87-550-3632-1
Original language: English (Risø-PhD: No. 33(EN)).
Keywords: Magnetic refrigeration, Numerical simulation, Cyclical steady state, Active Magnetic Regenerator (AMR), 2-D mathematical model, Experimental validation, Risø-PhD-33(EN), Risø-PhD-33, Risø-PhD-0033
Electronic versions:
TFPE_PhD_report_final.pdf
Source: orbit
Source-ID: 208018
Research output: Research › Ph.D. thesis – Annual report year: 2008

A versatile magnetic refrigeration test device
A magnetic refrigeration test device has been built and tested. The device allows variation and control of many important experimental parameters, such as the type of heat transfer fluid, the movement of the heat transfer fluid, the timing of the refrigeration cycle, and the magnitude of the applied magnetic field. An advanced two-dimensional numerical model has previously been implemented in order to help in the optimization of the design of a refrigeration test device. Qualitative agreement between the results from model and the experimental results is demonstrated for each of the four different parameter variations mentioned above. (C) 2008 American Institute of Physics.

General information
State: Published
Management
Contributors: Bahl, C. R. H., Petersen, T. F., Pryds, N., Smith, A.
Pages: 093906
Publication date: 2008
Peer-reviewed: Yes

Publication information
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.32 SJR 0.585 SNIP 0.858
Web of Science (2017): Impact factor 1.428
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.2 SJR 0.703 SNIP 1.048
Web of Science (2016): Impact factor 1.515
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.11 SJR 0.686 SNIP 0.908
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.45 SJR 0.972 SNIP 1.261
Web of Science (2014): Indexed yes
Web of Science (2014): Impact factor 1.614
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.28 SJR 0.9 SNIP 1.099
Web of Science (2013): Indexed yes
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.45 SJR 1.017 SNIP 1.277
Web of Science (2012): Indexed yes
Web of Science (2012): Impact factor 1.602
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.43 SJR 0.868 SNIP 1.108
Web of Science (2011): Indexed yes
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.218 SNIP 1.405
Web of Science (2010): Indexed yes
Web of Science (2010): Impact factor 1.601
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.001 SNIP 1.061
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.274 SNIP 1.344
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.922 SNIP 1.023
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.153 SNIP 1.297
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.883 SNIP 1.044
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.13 SNIP 1.393
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.994 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.02 SNIP 1.015
Scopus rating (2001): SJR 1.13 SNIP 1.301
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.022 SNIP 1.051
Comparison between a 1D and a 2D numerical model of an active magnetic regenerative refrigerator

The active magnetic regenerator (AMR) refrigeration system represents an environmentally attractive alternative to vapour-compression refrigeration. This paper compares the results of two numerical AMR models: (1) a 1D finite difference model and (2) a 2D finite element model. Both models simulate a reciprocating AMR and can determine the cyclical steady-state temperature profile of the system as well as performance parameters such as the refrigeration capacity, the work input and the coefficient of performance (COP). The models are used to analyse an AMR with a regenerator made of flat parallel plates of gadolinium operating in the presence of a 1 T magnetic field. The results are used to discuss under which circumstances a 1D model is insufficient and a 2D model is necessary. The results indicate that when the temperature gradients in the AMR perpendicular to the flow are small a 1D model obtains accurate results of overall results such as the refrigeration capacity but that a 2D model is required for a detailed analysis of the phenomena occurring inside the AMR.

General information

State: Published
Contributors: Petersen, T. F., Engelbrecht, K., Bahl, C. R. H., Elmegaard, B., Pryds, N., Smith, A.
Publication date: 2008
Peer-reviewed: Yes

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ISSN (Print): 0022-3727
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Impact factor 2.373
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Impact factor 2.588
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.1 SJR 0.886 SNIP 1.25
Web of Science (2015): Impact factor 2.772
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.53 SJR 1.096 SNIP 1.408
Web of Science (2014): Impact factor 2.721
Design of optical reflectance signals for wear control by varying the thickness of thin films of Ti-compounds

General information
State: Published
Organisations: Optical Microsensors and Micromaterials, Department of Photonics Engineering, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Rise National Laboratory for Sustainable Energy, CemeCon Scandinavia A/S
Energy efficient and environmentally friendly cooling using magnetic refrigeration

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Publication date: 2008
Peer-reviewed: No
Source: orbit
Source-ID: 222872
Research output: Research - peer-review › Journal article – Annual report year: 2008

Growth of thin films of TiN on MgO(100) monitored by high-pressure RHEED

Reflection high-energy electron diffraction (RHEED) operated at high pressure has been used to monitor the initial growth of titanium nitride (TiN) thin films on single-crystal (100) MgO substrates by pulsed laser deposition (PLD). This is the first RHEED study where the growth of TiN films is produced by PLD directly from a TiN target. At the initial stage of the growth (average thickness similar to 2.4 nm) the formation of islands is observed. During the continuous growth the islands merge into a smooth surface as indicated by the RHEED, atomic force microscopy and field emission scanning electron microscopy. These observations are in good agreement with the three-dimensional Volmer-Weber growth type, by which three-dimensional crystallites are formed and later cause a continuous surface roughening. This leads to an exponential decrease in the intensity of the specular spot in the RHEED pattern as well.

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Electroceramics, Optical Microsensors and Micromaterials, Department of Photonics Engineering, Technical University of Denmark
Pages: 705-710
Publication date: 2008
Peer-reviewed: Yes

Publication information
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ISSN (Print): 0947-8396
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.62 SJR 0.481 SNIP 0.699
Web of Science (2017): Impact factor 1.604
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.52 SJR 0.508 SNIP 0.744
Web of Science (2016): Impact factor 1.455
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.38 SJR 0.519 SNIP 0.768
Web of Science (2015): Impact factor 1.444
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.74 SJR 0.62 SNIP 0.965
Web of Science (2014): Impact factor 1.704
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.75 SJR 0.732 SNIP 1.01
Web of Science (2013): Impact factor 1.694
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.71 SJR 0.843 SNIP 1.033
Web of Science (2012): Impact factor 1.545
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.77 SJR 0.871 SNIP 1.119
Web of Science (2011): Impact factor 1.63
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.07 SNIP 1.025
Web of Science (2010): Impact factor 1.765
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.013 SNIP 0.988
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.203 SNIP 1.047
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.223 SNIP 1.081
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.301 SNIP 1.076
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.127 SNIP 0.924
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.13 SNIP 1.101
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.955 SNIP 0.905
Indirect measurement of the magnetocaloric effect using a novel differential scanning calorimeter with magnetic field

A simple and high-sensitivity differential scanning calorimeter (DSC) unit operating under magnetic field has been built for indirect determination of the magnetocaloric effect. The principle of the measuring unit in the calorimeter is based on Peltier elements as heat flow sensors. The high sensitivity of the apparatus combined with a suitable calibration procedure allows very fast and accurate heat capacity measurements under magnetic field to be made. The device was validated from heat capacity measurements for the typical DSC reference material gallium (Ga) and a La0.67Ca0.33MnO3 manganite system and the results were highly consistent with previous reported data for these materials. The DSC has a working range from 200 to 340 K and has been tested in magnetic fields reaching 1.8 T. The signal-to-noise ratio is in the range of 102–103 for the described experiments. Finally the results have been compared to results from a Quantum Design® physical properties measuring system. The configuration of the system also has the advantage of being able to operate with other types of magnets, e.g., permanent magnets or superconducting coils, as well as the ability to be expanded to a wider temperature range. ©2008 American Institute of Physics

General information
State: Published
Contributors: Jeppesen, S., Linderoth, S., Pryds, N., Kuhn, L. T., Jensen, J. B.
Pages: 083901
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Review of Scientific Instruments
Volume: 79
Issue number: 8
ISSN (Print): 0034-6748
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.32 SJR 0.585 SNIP 0.858
Web of Science (2017): Impact factor 1.428
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.2 SJR 0.703 SNIP 1.048
Web of Science (2016): Impact factor 1.515
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.11 SJR 0.686 SNIP 0.908
Web of Science (2015): Impact factor 1.336
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.45 SJR 0.972 SNIP 1.261
Web of Science (2014): Impact factor 1.614
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Numerical modeling of parallel-plate based AMR

In this work we present an improved 2-dimensional numerical model of a parallel-plate based AMR. The model includes heat transfer in fluid and magnetocaloric domains respectively. The domains are coupled via inner thermal boundaries. The MCE is modeled either as an instantaneous change between high and low field or as a magnetic field profile including the actual physical movement of the regenerator block in and out of field, i.e. as a source term in the thermal equation for the magnetocaloric material (MCM). The model is further developed to include parasitic thermal losses throughout the bed in the direction not resolved through a realistic description of the thermal resistance between localized points in the bed and the ambient. The results show that the additions to the model place numerical modeling of AMR very close to the corresponding experimental results. Thus, the model is verified by direct comparison with experiment. This is used as a firm basis for predicting and optimizing performance of a large variety of regenerator configurations in order to study and learn the trends, tendencies and even absolute values of temperature span and cooling powers for the optimal (and buildable) designs.

Optimization and Improvement of Halbach cylinder design

In this paper we describe the results of a parameter survey of a 16 segmented Halbach cylinder in three dimensions in which the parameters internal radius, rin, external radius, rex, and length, L, have been varied. Optimal values of rex and L were found for a Halbach cylinder with the least possible volume of magnets with a given mean flux density in the cylinder bore. The volume of the cylinder bore could also be significantly increased by only slightly increasing the volume of the magnets, for a fixed mean flux density. Placing additional blocks of magnets on the end faces of the Halbach cylinder also improved the mean flux density in the cylinder bore, especially so for short Halbach cylinders with large rex. Moreover, magnetic cooling as an application for Halbach cylinders was considered. A magnetic cooling quality parameter, LambdaCool, was introduced and results showed that this parameter was optimal for long Halbach cylinders with small rex. Using the previously mentioned additional blocks of magnets can improve the parameter by as much as 15% as well as improve the homogeneity of the field in the cylinder bore. ©2008 American Institute of Physics
**RHEED study of titanium dioxide using pulsed laser deposition**

General information
- State: Published
- Organisations: Risø National Laboratory for Sustainable Energy
- Contributors: Rasmussen, I., Pryds, N., Schou, J.
- Publication date: 2008
- Peer-reviewed: No
- Source: orbit
- Source-ID: 310095

Research output: Research › Conference abstract for conference – Annual report year: 2008

**RHEED Study of Titanium Dioxide Using Pulsed Laser Deposition**

General information
- State: Published
- Organisations: Optical Microsensors and Micromaterials, Department of Photonics Engineering, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
- Contributors: Rasmussen, I. L., Pryds, N., Schou, J.
- Publication date: 2008
- Peer-reviewed: No
- Source: orbit
- Source-ID: 224137

Research output: Research › Poster – Annual report year: 2008
Sintering behaviour of (La, Ca, Sr)\(_{1-x}\)MnxO3 as an active magnetic material sor magnetic refrigeration at room temperature

General information
State: Published
Organisations: Ceramic processing, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Thermo Ceramics
Contributors: Biering, I., Menon, M., Pryds, N.
Pages: 7-7
Publication date: 2008

Host publication information
Title of host publication: Book of abstracts
Publisher: American Ceramic Society
Source: orbit
Source-ID: 231984
Research output: Research › Conference abstract in proceedings – Annual report year: 2008

The liquid metastable miscibility gap in the Cu-Co-Fe system

General information
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Contributors: Curiotto, S., Battezzati, L., Johnson, E., Palumbo, M., Pryds, N.
Pages: 3253-3258
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Science
Volume: 43
ISSN (Print): 0022-2461
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.83 SJR 0.807 SNIP 1.064
Web of Science (2017): Impact factor 2.993
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.769 SNIP 1.072
Web of Science (2016): Impact factor 2.599
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.36 SJR 0.792 SNIP 1.059
Web of Science (2015): Impact factor 2.302
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.54 SJR 0.963 SNIP 1.388
Web of Science (2014): Impact factor 2.371
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.36 SJR 0.926 SNIP 1.451
Web of Science (2013): Impact factor 2.305
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 0.988 SNIP 1.383
Two-dimensional mathematical model of a reciprocating room-temperature Active Magnetic Regenerator

A time-dependent, two-dimensional mathematical model of a reciprocating Active Magnetic Regenerator (AMR) operating at room-temperature has been developed. The model geometry comprises a regenerator made of parallel plates separated by channels of a heat transfer fluid and a hot as well as a cold heat exchanger. The model simulates the different steps of the AMR refrigeration cycle and evaluates the performance in terms of refrigeration capacity and temperature span between the two heat exchangers. The model was used to perform an analysis of an AMR with a regenerator made of gadolinium and water as the heat transfer fluid. The results show that the AMR is able to obtain a no-load temperature span of 10.9 K in a 1 T magnetic field with a corresponding work input of 93.0 kJ m\(^{-3}\) of gadolinium per cycle. The model shows significant temperature differences between the regenerator and the heat transfer fluid during the AMR cycle. This indicates that it is necessary to use two-dimensional models when a parallel-plate regenerator geometry is used.

General information
State: Published
A numerical analysis of a reciprocating Active Magnetic Regenerator with a parallel-plate regenerator geometry

We have developed a two-dimensional model of a reciprocating Active Magnetic Regenerator (AMR) with a regenerator made of parallel plates arranged in a stack configuration. The time dependent, two-dimensional model solves the Navier-Stokes equations for the heat transfer fluid and the coupled heat transfer equations for the regenerator and the fluid. The model is implemented using the Finite Element Method. The model can be used to study both transient and steady-state phenomena in the AMR for any ratio of regenerator to fluid heat capacity. Results on the AMR performance for different design choices and operating parameters are presented and the implications for optimal AMR operation are discussed.

General information
State: Published
Contributors: Petersen, T. F., Pryds, N., Smith, A., Bahl, C. R. H.
Number of pages: 436
Pages: 271-279
Publication date: 2007

Host publication information
Title of host publication: Proceedings of the Second IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Volume: 1
Place of publication: Portoroz, Slovenia
Publisher: International Institute of Refrigeration
Edition: 1
ISBN (Print): 978-2-913149-56-4
Source: orbit
Source-ID: 197418
Research output: Research › Article in proceedings – Annual report year: 2007

A RHEED study of thin films grown on MgO samples by pulsed laser deposition

General information
State: Published
Contributors: Pryds, N., Cockburn, D., Rodrigo, K. A., Knudsen, J., Schou, J.
Publication date: 2007
Peer-reviewed: No
Event: Abstract from Danish Optical Society annual meeting 2007, Risø, Denmark.
URLs:
Source: orbit
Source-ID: 215763
Research output: Research › Conference abstract for conference – Annual report year: 2007
Atomic structure of glassy Mg60Cu30Y10 investigated with EXAFS, x-ray and neutron diffraction, and reverse Monte Carlo simulations

Short range order of amorphous Mg60Cu30Y10 was investigated by x-ray and neutron diffraction, Cu and Y K-edge x-ray absorption fine structure measurements, and the reverse Monte Carlo simulation technique. We found that Mg-Mg and Mg-Cu nearest neighbor distances are very similar to values found in crystalline Mg2Cu. The Cu-Y coordination number is 1.1 +/- 0.2, and the Cu-Y distance is similar to 4% shorter than the sum of atomic radii, suggesting that attraction between Cu and Y plays an important role in stabilizing the glassy state. Thermal stability and structure evolution upon annealing were also studied by differential scanning calorimetry and in situ x-ray powder diffraction. The alloy shows a glass transition and three crystallization events, the first and dominant one at 456 K corresponding to eutectic crystallization of at least three phases: Mg2Cu and most likely cubic MgY and CuMgY.
A tribological study of titanium nitrides with synchrotron radiation

General information
State: Published
Contributors: Rasmussen, I. L., Pedersen, H. C., Pryds, N., Schou, J., Mikkelsen, N., Feidenhans'l, R., Martin, J., Guibert, M., Belin, M.
Publication date: 2007
Peer-reviewed: No
Event: Abstract from 3rd Annual meeting Danish Physical Society, Nyborg, Denmark.

Characterization of lysozyme films produced by matrix assisted pulsed laser evaporation (MAPLE)
Thin lysozyme films of thickness up to more than 100 nm have been produced in a dry environment by MAPLE (matrix assisted pulsed laser evaporation) from a water ice matrix. Analysis of the films demonstrates that a significant part of the lysozyme molecules is transferred to the substrate without decomposition and that the protein activity is preserved. The film deposition rate for 1 wt% lysozyme has a maximum at 2 J/cm(2) of about 1 ng/cm(2) per laser shot. During the film production the deposition rate is constant without any sign of depletion or accumulation effects in the water ice target or in the growing film. Scanning electron microscopy (SEM) images demonstrate that the silicon substrate is completely covered by lysozyme films thicker than 100 nm. Deposition was also made from a target with pressed (100%) solid
lysozyme, but the deposition was difficult to handle and with a much slower rate than that from a water ice matrix. (C)
2007 Elsevier B.V. All rights reserved.

General information
State: Published
Contributors: Purice, A., Schou, J., Kingshott, P., Pryds, N., Dinescu, M.
Pages: 6451-6455
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
Web of Science (2013): Impact factor 2.538
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.26 SJR 0.913 SNIP 1.362
Web of Science (2012): Impact factor 2.112
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.922 SNIP 1.126
Web of Science (2010): Impact factor 1.795
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.84 SNIP 1.024
Characterization of yttria-stabilized zirconia thin films grown by pulsed laser deposition (PLD) on various substrates

General information
State: Published
Contributors: Rodrigo, K. A., Knudsen, J., Pryds, N., Schou, J., Linderoth, S.
Pages: 1338-1342
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
Volume: 254
Issue number: 4
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
Deposition of La0.8Sr0.2Cr0.97V0.03O3 and MnCr2O4 thin films on ferritic alloy for solid oxide fuel cell application

Single layer dense films of La0.8Sr0.2Cr0.97V0.03O3 (LSC) and MnCr2O4 with a thickness of 500 nm were deposited on a commercially available ferritic alloy (Crofer 22APU) by large-area Pulsed Laser Deposition. The deposited samples were subsequently oxidized at 1173 K for 500 h in humidified air. The effects of the deposited thin films on the growth rate and the morphology of the oxide were investigated by weight gain measurements as well as by scanning electron microscopy. The growth of the oxide scales was reduced by both coatings, and most effectively by the LSC coating. The overall
oxidation resistance and oxidation growth mechanism of the coated samples are discussed. (C) 2007 Elsevier B.V. All rights reserved.

**General information**
State: Published
Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Microstructures and Interfaces, Thermo Ceramics
Contributors: Mikkelsen, L., Chen, M., Hendriksen, P. V., Persson, Å. H., Pryds, N., Rodrigo, K. A.
Pages: 1262-1266
Publication date: 2007
Peer-reviewed: Yes

**Publication information**
Journal: Surface and Coatings Technology
Volume: 202
Issue number: 4-7
ISSN (Print): 0257-8972
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.08 SJR 0.928 SNIP 1.545
Web of Science (2017): Impact factor 2.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.882 SNIP 1.379
Web of Science (2016): Impact factor 2.589
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.46 SJR 0.852 SNIP 1.37
Web of Science (2015): Impact factor 2.139
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.44 SJR 0.983 SNIP 1.652
Web of Science (2014): Impact factor 1.998
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.58 SJR 1.048 SNIP 1.832
Web of Science (2013): Impact factor 2.199
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 1.041 SNIP 1.641
Web of Science (2012): Impact factor 1.941
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.38 SJR 1.041 SNIP 1.85
Web of Science (2011): Impact factor 1.867
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.145 SNIP 1.653
Web of Science (2010): Impact factor 2.141
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.441 SNIP 1.531
Effect of cooling rate on the solidification of Cu58Co42

General information
State: Published
Contributors: Curiotto, S., Pryds, N., Johnson, E., Battezzati, L.
Pages: 644-648
Publication date: 2007
Peer-reviewed: Yes

Publication information
Volume: 449-451
ISSN (Print): 0921-5093
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.76 SJR 1.694 SNIP 1.943
Web of Science (2017): Impact factor 3.414
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.669 SNIP 1.913
Web of Science (2016): Impact factor 3.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.01 SJR 1.742 SNIP 1.858
Web of Science (2015): Impact factor 2.647
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.32 SJR 2.235 SNIP 2.546
Web of Science (2014): Impact factor 2.567
Formation of thin films of yttria-stabilized zirconia thin films grown by pulse laser deposition (PLD) on various substrates

General information
State: Published
Growth dynamics of thin lysozyme films produced by matrix-assisted pulsed laser evaporation (MAPLE)

General information
State: Published
Contributors: Purice, A., Schou, J., Pryds, N., Filipescu, M., Dinescu, M.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 216340
Research output: Research › Paper – Annual report year: 2007

Growth of thin films of TiN on MgO(100) monitored by high pressure RHEED

General information
State: Published
Contributors: Pryds, N., Cockburn, D., Rodrigo, K. A., Rasmussen, I., Knudsen, J., Schou, J.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 215992
Research output: Research › Paper – Annual report year: 2007

High fluence deposition of polyethylene glycol films at 1064 nm by matrix assisted pulsed laser evaporation (MAPLE)
Matrix assisted pulsed laser evaporation (MAPLE) has been applied for deposition of thin polyethylene glycol (PEG) films with infrared laser light at 1064 nm. We have irradiated frozen targets (of 1 wt.% PEG dissolved in water) and measured the deposition rate in situ with a quartz crystal microbalance. The laser fluence needed to produce PEG films turned out to be unexpectedly high with a threshold of 9 J/cm(2) and the deposition rate was much lower than that with laser light at 355 nm. Results from matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) analysis demonstrate that the chemistry, molecular weight and polydispersity of the PEG films were identical to the starting material. Studies of the film surface with scanning electron microscopy (SEM) indicate that the Si-substrate is covered by a relatively homogenous PEG film with few bare spots. (c) 2007 Elsevier B.V. All rights reserved.

General information
State: Published
Contributors: Purice, A., Schou, J., Kingshott, P., Pryds, N., Dinescu, M.
Pages: 7952-7956
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
Volume: 253
Issue number: 19
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
Web of Science (2013): Impact factor 2.538
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.26 SJR 0.913 SNIP 1.362
Web of Science (2012): Impact factor 2.112
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.922 SNIP 1.126
Web of Science (2010): Impact factor 1.795
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.84 SNIP 1.024
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.89 SNIP 1.084
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.791 SNIP 0.935
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.861 SNIP 1.046
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.689 SNIP 0.938
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.984 SNIP 1.123
Scopus rating (2003): SJR 1.017 SNIP 1.036
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.954 SNIP 0.97
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.874 SNIP 0.804
Indirect measurement of the magnetocaloric effect using a novel DSC with magnetic field

General information
State: Published
Contributors: Jeppesen, S., Linderoth, S., Pryds, N., Kuhn, L.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 216345
Research output: Research - peer-review › Paper – Annual report year: 2007

Large-area production of yttria-stabilized zirconia by pulsed laser deposition

General information
State: Published
Contributors: Pryds, N., Schou, J., Linderoth, S.
Pages: 140-143
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Journal of Physics: Conference Series (Online)
Volume: 59
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.48 SJR 0.241 SNIP 0.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.35 SJR 0.252 SNIP 0.374
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.32 SJR 0.264 SNIP 0.352
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.25 SJR 0.245 SNIP 0.293
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Magnetic cooling for use in refrigerators

General information
State: Published
Publication date: 2007
Peer-reviewed: No
Event: Abstract from 3rd Annual meeting Danish Physical Society, Nyborg, Denmark.
URLs:
Source: orbit
Source-ID: 215988
Research output: Research › peer-review › Conference article – Annual report year: 2007

Optical monitoring of abrasive wear of titanium compounds in tribological hard coatings

General information
State: Published
Contributors: Rasmussen, I. L., Pedersen, H., Schou, J., Pryds, N.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 216341
Research output: Research › Paper – Annual report year: 2007

Phase separation of undercooled copper alloy

General information
Preparation of La0.8Sr0.2Cr0.97V0.03O3-delta films for solid oxide fuel cell application

La0.8Sr0.2Cr0.97V0.03O3-delta (LSC) is commonly studied as a ceramic interconnect material as well as a coating material for metallic interconnects for solid oxide fuel cell applications. However, it is difficult to sinter this type of material to high density. In order to overcome this problem and to study the material in form of a thin film we have used Pulsed Laser Deposition to obtain a dense, uniform film with the right stoichiometry. Investigation of preparation-parameter dependence of the LSC films deposited on a stainless steel substrate during pulsed-laser deposition was carried out. The LSC films were deposited with KrF excimer laser (248 nm) on a stainless steel substrate at different oxygen pressure and substrate temperatures. The substrate temperature (873-1073 K) and the oxygen background pressure (5-20 Pa) were varied in order to obtain optimal growth conditions. The surface morphology and structural information of the films were obtained using scanning electron microscope (SEM) and X-ray diffraction, respectively. Under the optimal preparation-parameter conditions: substrate temperature of 1023 K and an oxygen pressure of 10 Pa the structure of the film agreed with the target structure and the SEM micrographs show that the surfaces are homogeneous, smooth, crack-free and dense. (C) 2006 Elsevier B.V. All rights reserved.
Surface morphology of thin lysozyme films produced by matrix-assisted pulsed laser evaporation (MAPLE)

Thin films of the protein, lysozyme, have been deposited by the matrix-assisted pulsed laser evaporation (MAPLE) technique. Frozen targets of 0.3-1.0 wt.% lysozyme dissolved in ultrapure water were irradiated by laser light at 355 nm with a fluence of 2 J/cm². The surface quality of the thin lysozyme films of different thickness deposited on 7 rum x 7 turn Si-(1 0 0) -wafers was investigated with scanning electron microscopy and atomic force microscopy. Already at comparatively low thickness, similar to 20 nm, the substrate is covered by intact lysozyme molecules and fragments. The concentration of lysozyme in the ice matrix apparently does not play any significant role for the morphology of the film. The morphology obtained with MAPLE has been compared with results for direct laser irradiation of a pressed lysozyme
sample (i.e. pulsed laser deposition (PLD)). (C) 2007 Elsevier B.V. All rights reserved.

**General Information**

State: Published
Contributors: Purice, A., Schou, J., Pryds, N., Filipescu, M., Dinescu, M.
Pages: 1244-1248
Publication date: 2007
Peer-reviewed: Yes

**Publication Information**

Journal: APPLIED SURFACE SCIENCE
Volume: 254
Issue number: 4
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
Web of Science (2013): Impact factor 2.538
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.26 SJR 0.913 SNIP 1.362
Web of Science (2012): Impact factor 2.112
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.922 SNIP 1.126
Web of Science (2010): Impact factor 1.795
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.84 SNIP 1.024
The liquid metastable miscibility gap in Cu-based systems

Some Cu-based alloys, like Cu–Co, Cu–Fe and Cu–Co–Fe, display a liquid metastable miscibility gap. When the melt is undercooled below a certain temperature depending on the alloy composition, they present a separation in two liquid phases, followed by coagulation before dendritic solidification. In order to predict the phase equilibria and the mechanisms of microstructure formation, a determination of the metastable monotectics in the phase diagrams is essential. This paper focuses on the up-to-date findings on the Cu–Co, Cu–Fe and Cu–Co–Fe metastable miscibility gap in the liquid phase. Furthermore, the knowledge on the phase equilibria in the three systems is extended by presenting new results obtained by differential scanning calorimetry (DSC) and comparing them with the calculated phase diagrams.
Thermodynamics and mechanism of demixing in undercooled CU-Co-Ni alloys

General information
State: Published
Contributors: Curiotto, S., Battezzati, L., Johnson, E., Pryds, N.
Pages: 6642-6650
Publication date: 2007
Peer-reviewed: Yes

Publication information
Volume: 55
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Impact factor 6.036
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Impact factor 5.301
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.22 SJR 3.417 SNIP 2.831
Web of Science (2015): Impact factor 5.058
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.16 SJR 3.885 SNIP 3.166
Web of Science (2014): Impact factor 4.465
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.37 SJR 3.238 SNIP 2.674
Web of Science (2013): Impact factor 3.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.28 SJR 3.37 SNIP 2.875
Web of Science (2012): Impact factor 3.941
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.27 SJR 3.215 SNIP 2.768
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.709 SNIP 2.698
Web of Science (2010): Impact factor 3.791
Web of Science (2010): Indexed yes
The spatial thickness distribution of metal films produced by large area pulsed laser deposition

Thin films of metals have been deposited in the large-area Pulsed Laser Deposition (PLD) Facility at Riso National Laboratory. Thin films of Ag and Ni were deposited with laser pulses from an excimer laser at 248 nm with a rectangular beam spot at a fluence of 10 J/cm\(^2\) on glass substrates of 127 mm diameter positioned 80 turn from the target in vacuum. We have explored the distribution of deposited material on a stationary substrate from a fixed point of impact on the target relative to the substrate. In all cases the angular distribution of the deposited metal layers shows a distinct "flip-over" of the plume. The thickness of the deposited films over the full area has been determined by energy-dispersive X-ray spectrometry in a scanning electron microscope (SEM). The measured distributions were then compared with analytical expressions. Finally, the angular distribution of the film thickness has been utilized in an algorithm for production of films over large areas. (c) 2007 Elsevier B.V. All rights reserved.

General information
State: Published
Contributors: Pryds, N., Schou, J., Linderoth, S.
Pages: 8231-8234
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
Volume: 23
Issue number: 19
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Impact factor 4.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Impact factor 3.387
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.13 SJR 0.89 SNIP 1.268
Web of Science (2015): Impact factor 3.15
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.96 SJR 0.948 SNIP 1.453
Web of Science (2014): Impact factor 2.711
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.78 SJR 0.96 SNIP 1.475
Web of Science (2013): Impact factor 2.538
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.26 SJR 0.913 SNIP 1.362
Web of Science (2012): Impact factor 2.112
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.27 SJR 0.908 SNIP 1.386
Web of Science (2011): Impact factor 2.103
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.922 SNIP 1.126
Web of Science (2010): Impact factor 1.795
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.84 SNIP 1.024
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.89 SNIP 1.084
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.791 SNIP 0.935
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.861 SNIP 1.046
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.689 SNIP 0.938
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.984 SNIP 1.123
Scopus rating (2003): SJR 1.017 SNIP 1.036
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.954 SNIP 0.97
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.874 SNIP 0.804
Scopus rating (2000): SJR 1.065 SNIP 0.783
Thickness dependence of conductivity of thin films deposited on MgO single crystal

**General information**
State: Published
Organisations: Electroceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Mosleh, M., Pryds, N., Hendriksen, P.
Publication date: 2007
Peer-reviewed: No

**Thickness dependence of the conductivity of thin films (La, Sr)FeO$_3$ deposited on MgO single crystal**

Thin films of La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$ of different thicknesses have been deposited on single crystal MgO substrate by pulsed laser deposition (PLD). The deposited films are characterized by XRD before and after annealing, by scanning electron microscopy (SEM) for morphological characterization and by the Van der Pauw (VDP) technique for determination of the conductivity. The temperature dependence of the conductivity in air for samples of different thickness has been investigated. The electrical conductivity of the films increases with increasing film thickness but the conductivity of all films is less than the value of the bulk material. The apparent conductivity versus temperature shows a maximum at a certain temperature (T-max). This characteristic temperature (T-max) decreases as the film thickness increases and reaches the value for bulk for thicker films. All of the samples show the same activation energy of the conductivity in the low temperature limit. (C) 2007 Elsevier B.V. All rights reserved.
Undercooling and demixing in rapidly solidified Cu-Co alloys

The Cu–Co system displays a metastable miscibility gap in the liquid state. A considerable amount of work has been performed to study phase separation and related microstructures showing that demixing of the liquid is followed by coagulation before dendritic solidification. Due to kinetic competition of transformation phenomena, the mechanisms have not been fully disclosed.

This contribution reviews such findings with the help of a computer calculation of the phase diagram and extends the present knowledge by presenting new results obtained by rapidly solidifying various Cu–Co compositions using a wide range of cooling rates achieved by forcing the liquid into cylindric and conic moulds and by melt spinning.

General information

State: Published
Contributors: Battezzati, L., Curiotto, S., Johnson, E., Pryds, N.
Pages: 7-11

DOI: 10.1016/j.mseb.2007.07.089
Source: orbit
Source-ID: 215823
Research output: Research - peer-review › Journal article – Annual report year: 2007
Deposition of polyethylene glycol films (PEG) by matrix assisted pulsed laser evaporation (MAPLE) using infrared light

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Purice, A., Schou, J., Kingshott, P., Pryds, N., Dinescu, M.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from Danish Physical Society Annual Meeting 2006, Nyborg, Denmark.
Source: orbit
Source-ID: 309478
Research output: Research › Conference abstract for conference – Annual report year: 2006

High fluence deposition of polyethylene glycol films at 1064 nm by matrix assisted pulsed laser evaporation (MAPLE)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Purice, A., Schou, J., Kingshott, P., Pryds, N., Dinescu, M.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from European Materials Research Society Spring 2006 meeting, Nice, France.
Source: orbit
Source-ID: 309344
Research output: Research › Conference abstract for conference – Annual report year: 2006

High-quality protein films produced by Maple (Matrix assisted pulsed laser evaporation)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Purice, A., Schou, J., Kingshott, P., Pryds, N., Disnescu, M.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 5. International conference on photo-excited processes and applications (ICPEPA 5), Charlottesville, VA (US), 3-7 Sep.,
Source: orbit
Source-ID: 309540
Research output: Research › Conference abstract for conference – Annual report year: 2006
Large area metal films produced by pulsed laser deposition

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Schou, J., Linderoth, S.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from European Materials Research Society Spring 2006 meeting, Nice, France.
Source: orbıt
Source-ID: 309342
Research output: Research › Conference abstract for conference – Annual report year: 2006

Large area pulse laser deposition

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from Keramiske belægninger. Temadag i samarbejde mellem Dansk Keramisk Selskab og Dansk Metallurgisk Selskab, Risø (DK), 7 Jun, .
Source: orbıt
Source-ID: 309309
Research output: Research › Conference abstract for conference – Annual report year: 2006

Liquid-liquid phase separation and remixing in the Cu-Co system

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division
Contributors: Curiotto, S., Pryds, N., Johnson, E., Battezzati, L.
Pages: 2361-2368
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science
Volume: 37 A
ISSN (Print): 1073-5623
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.08 SJR 1.093 SNIP 1.28
Web of Science (2017): Impact factor 1.887
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.91 SJR 1.206 SNIP 1.336
Web of Science (2016): Impact factor 1.874
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.78 SJR 1.267 SNIP 1.407
Web of Science (2015): Impact factor 1.749
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.06 SJR 1.659 SNIP 1.848
Web of Science (2014): Impact factor 1.73
Web of Science (2014): Indexed yes
Magnetic Refrigeration and the Magnetocaloric Effect

Magnetic refrigeration at room temperature is an emerging technology for refrigeration, which promises low energy consumption and is environmentally friendly. Magnetic refrigeration is based on the magnetocaloric effect, which manifests itself as a reversible increase in temperature when magnetic material are placed in a magnetic field. This paper introduces and describes magnetic refrigeration cycles and the magnetocaloric effect, and shows how magnetic refrigeration can be an alternative to vapour-compression refrigeration. A review of the Danish research on magnetic refrigeration at Risø National Laboratory is also provided.
Optical control of tribological nanothinfilms: A wear sensor

Preparation of La_{1-x}Sr_{x}CrO_{3-δ} films for Solid Oxide Fuel Cell (SOFC) application

Protein films produced by Maple (Matrix assisted pulsed laser evaporation)

The liquid metastable miscibility gap in Cu-based systems
Thickness determination of large-area films of yttria-stabilized zirconia produced by pulsed laser deposition

Films of yttria-stabilized zirconia (YSZ) on a polished silicon substrate of diameter up to 125 mm have been produced in a large-area pulsed laser deposition (PLD) setup under typical PLD conditions. The film thickness over the full film area has been determined by energy-dispersive X-ray spectrometry in a scanning electron microscope (SEM) with use of a method similar to one described by Bishop and Poole. The attenuation of the electron-induced X-rays from the Si wafer by the film was monitored at a number of points along a diameter and the thickness was determined by Monte Carlo simulations of the attenuation for various values of film thickness with the program CASINO. These results have been compared with direct measurements in the SEM of the film thickness on a cross-section on one of the wafers. The results of these measurements demonstrate the ability of this technique to accurately determine the thickness of a large film, i.e. up to diameters of 125 mm, in a relatively short time, without destroying the substrate, without the need of a standard sample and without the need of a flat substrate. We have also demonstrated that by controlling the deposition parameters large-area YSZ films with uniform thickness can be produced. (c) 2005 Elsevier B.V. All rights reserved.
Undercooling and demixing of copper-based alloys

Since the beginning of materials science research under microgravity conditions immiscible alloys have been an interesting subject. New possibilities to investigate such systems are offered by containerless processing techniques. Of particular interest is the ternary system Cu-Fe-Co, and its limiting binaries, Cu-Co and Cu-Fe. They all show a metastable miscibility gap in the regime of the undercooled melt. Within the ESA-MAP project “CoolCop”, different aspects of this alloy have been investigated; results obtained so far are reported here.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 174-177
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Microgravity - Science and Technology
Volume: 18
Issue number: 3-4
Using a Linux Cluster for Parallel Simulations of an Active Magnetic Regenerator Refrigerator
This paper describes the implementation of a Comsol Multiphysics model on a Linux computer Cluster. The Magnetic Refrigerator (MR) is a special type of refrigerator with potential to reduce the energy consumption of household refrigeration by a factor of two or more. To conduct numerical analysis of an experimental MR, a mathematical model was developed. The model solves the coupled Navier-Stokes and heat transfer equations which describe the physical phenomenon occurring within the MR. The MR performs a cyclic process, and the model must be time-dependent to determine the steady-state conditions. The coupled set of equations and the transient convergence towards the final steady state means that the model has an excessive solution time. To make parametric studies practical, the developed model was implemented on a Cluster to allow parallel simulations, which has decreased the solution time significantly.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Petersen, T., Pryds, N., Smith, A.
Number of pages: 150
Pages: 129-134
Publication date: 2006

Host publication information
Title of host publication: Proceedings of the Nordic COMSOL Conference 2006
Volume: 1
Place of publication: Lyngby
Publisher: COMSOL A/S
Editor: Gregersen, L.
Edition: 1st
ISBN (Print): 87-989426-1-1
Source: orbit
Source-ID: 194748
Research output: Research - peer-review › Article in proceedings – Annual report year: 2006

Wear control of tribological hard coatings with embedded optical nano-layers

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Rasmussen, I., Pryds, N., Pedersen, H., Schou, J.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from Danish Physical Society Annual Meeting 2006, Nyborg, Denmark.
Source: orbit
Source-ID: 309477
Research output: Research › Conference abstract for conference – Annual report year: 2006

Co precipitate sites in Cu$_{0.90}$Co$_{0.10}$ and their relation to magnetoresistance (poster)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Andreasen, J., Jeppesen, S., Andreasen, A., Xu, M., Pryds, N.
Publication date: 2005
Peer-reviewed: No
Event: Poster session presented at HASYLAB users meeting, Hamburg, Germany.
Source: orbit
Source-ID: 307798
Research output: Research › Poster – Annual report year: 2005

Effect of cooling rates on the microstructure in Cu-Co alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Curiotto, S., Pryds, N., Johnson, E., Battezzati, L.
Publication date: 2005
Peer-reviewed: No
Electrical and structural properties of La$_{0.8}$Sr$_{0.2}$Mn$_{0.5}$Co$_{0.5}$O$_{3+\delta}$ films produced by pulsed laser deposition

La$_{0.8}$Sr$_{0.2}$Mn$_{0.5}$Co$_{0.5}$O$_3$ (LSMCO) films for the use as contact layers or protective coatings in solid oxide fuel cells (SOFC) have been deposited on glass substrates by pulsed laser deposition (PLD). PLD is an obvious technique for thin film production of complex oxides, because of the ability to transfer material stoichiometrically from a multicomponent target to a growing film. In the present study, films were deposited at substrate temperatures of 473 and 573 K and in different oxygen background pressures. The influence of the process parameters, in particular of the oxygen background gas pressure, on the electrical conductivity and structure of the films is investigated. (c) 2005 Elsevier B.V. All rights reserved.
Fundamentals of Numerical Modelling of Casting Processes

Fundamentals of Numerical Modelling of Casting Processes comprises a thorough presentation of the basic phenomena that need to be addressed in numerical simulation of casting processes. The main philosophy of the book is to present the topics in view of their physical meaning, whenever possible, rather than relying strictly on mathematical formalism. The book, aimed both at the researcher and the practicing engineer, as well as the student, is naturally divided into four parts. Part I (Chapters 1-3) introduces the fundamentals of modelling in a 1-dimensional framework. Part II (Chapter 4) presents the most important aspects of solidification theory related to modelling. Part III (Chapter 5) describes the fluid flow phenomena and in part IV (Chapter 6) the stress-strain analysis is addressed. For all parts, both numerical formulations as well as some important analytical solutions are presented. As a very deliberate choice, all the numerical formulations in the book are developed in the same framework based on the Finite Volume Method (FVM). This makes the differences and similarities between the formulations of solidification, fluid flow and stress-strain problems transparent and clear.

General information
State: Published
Organisations: Department of Management Engineering, Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Magma Gießereitechnologie GmbH
Number of pages: 540
Publication date: 2005

Publication information
Publisher: Polyteknisk Forlag
ISBN (Print): 8750209698
Original language: English
Source: orbit
Large-scale production of yttria-stabilized zirconia by pulsed laser deposition

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Schou, J., Linderoth, S.
Publication date: 2005
Peer-reviewed: No
Event: Abstract from 8th International Conference on Laser Ablation, Banff, Canada.
Source: orbit
Source-ID: 308366
Research output: Research › Conference abstract for conference – Annual report year: 2005

Large-scale pulsed laser deposition (poster)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Schou, J., Linderoth, S.
Publication date: 2005
Peer-reviewed: No
Event: Poster session presented at Annual meeting of the Danish Optical Society 2005, Roskilde, Denmark.
URLs:
Source: orbit
Source-ID: 308549
Research output: Research › Poster – Annual report year: 2005

On the development of amorphous alloy using rapid solidification processes

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Pages: 185-198
Publication date: 2005

Host publication information
Title of host publication: Stærkning og støbning
Place of publication: Lyngby
Publisher: DMS
Editor: Somers, M.
ISBN (Print): 87-97535-34-3
Source: orbit
Source-ID: 307922
Research output: Research › Article in proceedings – Annual report year: 2005

Spray forming: A numerical investigation of the influence of the gas to melt ratio on the billet surface temperature
The relationship between the Gas to Melt Ratio (GMR) and the surface temperature of an evolving billet surface in spray forming is investigated numerically. The basis for the analysis is an integrated approach for modelling the entire spray forming process. This model includes the droplet atomisation taking thermal coupling into consideration and the deposition of material at the surface of the billet taking geometrical aspects such as shading into account. The coupling between these two models is accomplished by ensuring that the total droplet size distribution of the spray is the summation of "local" droplet size distributions along the r-axis of the spray cone. The criterion for a successful process has been a predefined process window characterised by a desired fraction solid range at a certain distance from the atomizer. Inside this process window, the gas and melt flows have been varied and the influence of the gas and metal flow rates on the surface temperature of the billet has been analysed. Based on this, a relationship for the surface temperature as function of the GMR has been suggested for the spray forming of a 100Cr6 billet.

General information
Thickess determination of large-area films of yttria-stabilized zirconia produced by pulsed laser ablation

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Christensen, B. T., Bilde-Sørensen, J., Schou, J., Linderoth, S.
Publication date: 2005
Peer-reviewed: No
Source: orbit
Source-ID: 308093
Research output: Research › Conference abstract for conference – Annual report year: 2005

Undercooling and demixing in rapidly solidified Cu-Co alloys

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Battezzati, L., Curiotto, S., Johnson, E., Pryds, N.
Publication date: 2005
Peer-reviewed: No
Event: Abstract from 12th International Meeting on Rapidly Quenched Materials, Seoul, Korea, Republic of.
Source: orbit
Source-ID: 308321
Research output: Research › Conference abstract for conference – Annual report year: 2005

Undercooling and demixing of copper-based alloys

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Publication date: 2005
Peer-reviewed: No
Event: Abstract from ELGRA biennial symposium and general assembly, Santorini (GR), 21-23 Sep, .
Source: orbit
Source-ID: 308568
Research output: Research › Conference abstract for conference – Annual report year: 2005

Undercooling and demixing of copper-based alloys

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Curiotto, S., Pryds, N., Johnson, E., Battezzati, L.
Publication date: 2005
Peer-reviewed: No
Event: Abstract from 3rd Annual Meeting in the Copenhagen Graduate School for Nanoscience and Nanotechnology, Copenhagen, Denmark.
URLs:
http://www.risoe.dtu.dk/rispubl/AFM/afmpdf/afm_5_2006.pdf
Bulk amorphous Mg-based alloys

The present paper describes the preparation and properties of bulk amorphous quarternary Mg-based alloys and the influence of additional elements on the ability of the alloy to form bulk amorphous. The main goal is to find a Mg-based alloy system which shows both high strength to weight ratio and a low glass transition temperature. The alloys were prepared by using a relatively simple technique, i.e. rapid cooling of the melt in a copper wedge mould. The essential structural changes that are achieved by going from the amorphous to the crystalline state through the supercooled liquid state are discussed in this paper. On the basis of these measurements phase diagrams of the different systems were constructed. Finally, it is demonstrated that when pressing the bulk amorphous alloy onto a metallic dies at temperatures within the supercooled liquid region, the alloy faithfully replicates the surface topology of dies with patterns smaller than 1 mum, suggesting potential applications in devices with submicrometer-scale features. (C) 2003 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Pages: 186-193
Publication date: 15 Jul 2004
Peer-reviewed: Yes

Publication information
Volume: 375-377
Issue number: SI
ISSN (Print): 0921-5093
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.76 SJR 1.694 SNIP 1.943
Web of Science (2017): Impact factor 3.414
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.669 SNIP 1.913
Web of Science (2016): Impact factor 3.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.01 SJR 1.742 SNIP 1.858
Web of Science (2015): Impact factor 2.647
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.32 SJR 2.235 SNIP 2.546
Web of Science (2014): Impact factor 2.567
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.86 SJR 1.868 SNIP 2.235
Web of Science (2013): Impact factor 2.409
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.5 SJR 1.744 SNIP 2.358
Web of Science (2012): Impact factor 2.108
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.59 SJR 1.74 SNIP 2.414
Web of Science (2011): Impact factor 2.003
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.723 SNIP 2.114
Web of Science (2010): Impact factor 2.101
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.57 SNIP 1.757
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.682 SNIP 1.859
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.326 SNIP 1.701
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.337 SNIP 1.756
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.201 SNIP 1.444
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.288 SNIP 1.625
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.42 SNIP 1.632
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.413 SNIP 1.368
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.157 SNIP 1.391
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.083 SNIP 1.084
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.168 SNIP 1.072
Original language: English
Keywords: bulk amorphous alloy, Mg-alloy, glass transition, mechanical properties, glass-forming ability
DOIs:
10.1016/j.msea.2003.10.147
Source: orbit
Source-ID: 306996
Research output: Research - peer-review › Conference article – Annual report year: 2004

Conductive and protective properties of La$_{0.8}$Sr$_{0.2}$Mn$_{0.5}$Co$_{0.5}$O$_3$ films produced by pulsed laser deposition

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Christensen, B. T., Schou, J., Hendriksen, P., Linderoth, S.
Publication date: 2004
Peer-reviewed: No
Source: orbit
Source-ID: 307430
Research output: Research › Conference abstract for conference – Annual report year: 2004

Co precipitate sizes in Cu$_{0.90}$Co$_{0.10}$ and their relation to magnetoresistance (poster)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Andreasen, J., Jeppesen, S., Andreasen, A., Pryds, N.
Deformation characteristics of Mg_{60}Cu_{30}Y_{10} alloy at temperatures near T_g.

The mechanical behaviour of nanocrystallized samples with a crystalline volume fraction of 15%, 50%, 75% and 100% was investigated by constant compression rate tests at different strain rates at 430 K and shows an increase in yield or flow stress provided that their crystalline volume fraction were less than 50%. (C) 2004 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
Dependence of magnetoresistance on the particle size distribution of Co clusters in phase-separated Cu$_{90}$Co$_{10}$

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Andreasen, J., Jeppesen, S., Pryds, N.
Publication date: 2004

Host publication information
Title of host publication: HASYLAB annual report 2003. Part 1
Place of publication: Hamburg
Publisher: HASYLAB
URLs:
Source: orbit
Source-ID: 306554
Research output: Communication › Book chapter – Annual report year: 2004

Kan et metal være en glas?

General information
Structure, annealing characteristics and mechanical properties of Mg₆₀Cu₃₀₋ₓY₁₀Siₓ bulk amorphous alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wolff, U., Yang, B., Pryds, N., Wert, J. A.
Pages: 287-292
Publication date: 2004

Host publication information
Title of host publication: Supercooled liquids, glass transition and bulk metallic glasses
Place of publication: Warrendale
Publisher: Materials Research Society
Editors: Greer, A., Egami, T., Inoue, A., Ranganathan, S.
Source: orbit
Source-ID: 307427
Research output: Research › Article in proceedings – Annual report year: 2004

The effect of partial crystallization on elevated temperature flow stress and room temperature handness of a bulk amorphous Mg₆₀Cu₃₀Y₁₀ alloy

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 1989-1995
Publication date: 2004
Peer-reviewed: Yes

Publication information
Volume: 52
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Impact factor 6.036
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Impact factor 5.301
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.22 SJR 3.417 SNIP 2.831
Web of Science (2015): Impact factor 5.058
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.16 SJR 3.885 SNIP 3.166
Web of Science (2014): Impact factor 4.465
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.37 SJR 3.238 SNIP 2.674
Web of Science (2013): Impact factor 3.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.28 SJR 3.37 SNIP 2.875
Web of Science (2012): Impact factor 3.941
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.27 SJR 3.215 SNIP 2.768
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.709 SNIP 2.698
Web of Science (2010): Impact factor 3.791
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.663 SNIP 2.625
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.82 SNIP 2.774
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.615 SNIP 3.118
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.22 SNIP 3.038
Scopus rating (2004): SJR 3.308 SNIP 3.073
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.852 SNIP 3.258
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.198 SNIP 2.73
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 3.22 SNIP 2.164
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.069 SNIP 2.167

Original language: English
The local atomic structure of the Mg$_{60}$Cu$_{30}$Y$_{10}$ bulk amorphous alloy

Magnetocaloric and magnetoresistive properties of La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$

This thesis presents results of an experimental investigation of magnetocaloric and magnetoresistive properties of a series of polycrystalline Ca- and Sr-doped lanthanum manganites, La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$ (0<=x<=0.33), with the perovskite structure. The samples consisted of sintered oxide powders prepared by the glycine-nitrate combustion technique. The compounds were ferromagnetic and showed a Curie transition in the temperature range 267–370 K (TC increased with increasing x). An analysis of the structural properties was carried out by means of x-ray diffraction and the Rietveld technique. The variation of the Ca/Sr ratio was found to cause a transition from orthorhombic to rhombohedral symmetry in the composition range 0.110 <x <0.165. The analysis suggested a strong correlation between structural properties and magnetism, for instance a relationship between the mean Mn–O–Mn bond angle and the Curie temperature. The Mn–O–Mn bonds mediate ferromagnetism and electrical transport in these materials via the double-exchange mechanism.

The magnetocaloric effect of the La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$ samples was measured directly and indirectly (by means of magnetization measurements). All the samples showed a magnetocaloric effect in the vicinity of TC. A model for the magnetocaloric effect based on Weiss mean field theory and classical theories for heat capacities was developed. The model provided reasonable predictions of the magne-tocaloric properties of the samples. The compounds with low Sr content showed a magnetocaloric effect comparable to that of Gadolinium, the prototypical working material for magnetic refrigeration at room temperature. A less comprehensive part of the investigation regarded the magnetoresistive properties of the La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$ system. It was found that the polycrystalline nature of the compounds played a decisive role for the magnetotransport properties. Characteristic grain boundary effects, such as a low-field magnetoresistance, which is absent in single-crystalline perovskites, were observed. The low-field effect is usually ascribed to spin-dependent scattering in grain boundaries. Qualitatively the results obtained for the La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$ samples were consistent with this model. The resistivity contribution arising from the presence of grain boundaries increased with increasing Sr content. Reducing the sintering temperature also enhanced the grain boundary effects. The samples with low Sr content showed colossal magnetoresistance (CMR) near room temperature (~20-45 % with µ0H = 0.8 T). The CMR effect was negligible for the samples with high Sr content. However, these samples exhibited a grain boundary-related magnetoresistance at room temperature.
Crystallization of Cu₆₀Ti₂₀Zr₂₀ metallic glass with and without pressure

Structural stability of a Cu₆₀Ti₂₀Zr₂₀ metallic glass under-pressure up to 4.5 GPa was investigated by x-ray diffraction. The sample exhibited a supercooled liquid region of 33 K and a ratio of the glass-transition temperature to the liquidus temperature of 0.63. The glass crystallized in two-step transformation processes in the pressure range of 0-4.5 GPa; the first was a primary reaction to form a Cu₅₁Zr₁₄-type structure crystalline phase with a spacing group P₆/m (175) and lattice parameters a = 11.235 Angstrom and c = 8.271 Angstrom, and then the residual amorphous phase crystallized into a MgZn₂-type, structure crystalline phase with a spacing group P₆(3)/mmc (194) and lattice parameters a = 5.105 Angstrom and c = 8.231 Angstrom. Both crystallization temperatures increased with pressure having a slope of 19 K/GPa. The increase of the first crystallization temperature with increasing pressure in the glass can be explained by the suppression of atomic mobility. No significant structural change was detected in the Cu₆₀Ti₂₀Zr₂₀ glass annealed in vacuum at 697 K for 1 h as compared to the as-prepared sample from x-ray diffraction measurements.
Cycling effect on undercooling in Pd$_{40}$Cu$_{30}$Ni$_{10}$P$_{20}$ melt

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Linderoth, S., Jiang, J.
Pages: 87-92
Publication date: 2003
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Metastable and Nanocrystalline Materials
Volume: 15/16
ISSN (Print): 1422-6375
Ratings:
Scopus rating (2008): SJR 0.177 SNIP 0.217
Scopus rating (2007): SJR 0.271 SNIP 0.558
Scopus rating (2006): SJR 0.257 SNIP 0.519
Scopus rating (2005): SJR 0.247 SNIP 0.29
Scopus rating (2004): SJR 0.335 SNIP 0.497
Web of Science (2003): Indexed yes
Original language: English
Source: orbit
Source-ID: 305392
Magnetocaloric properties of La$_{0.67}$Ca$_{0.33-x}$Sr$_x$MnO$_3$+$\delta$

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Dinesen, A., Linderoth, S., Mørup, S., Pryds, N.
Pages: 49-50
Publication date: 2003

Host publication information
Title of host publication: Superconductivity and magnetism: Materials properties and developments. Extended abstracts
Place of publication: Roskilde
Publisher: Risø National Laboratory
ISBN (Print): 87-550-3244-3
URLs:
Source: orbit
Source-ID: 305809

Metallic glasses

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wert, J. A., Pryds, N.
Pages: 1-25
Publication date: 2003
Peer-reviewed: Unknown

Publication information
Journal: Materialenyt
Issue number: 1
Original language: English
Source: orbit
Source-ID: 306982

Numerical model for the prediction of Gaussian and Billet shape (invited paper)

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Hattel, J., Pryds, N., Pedersen, T.
Pages: 109-116
Publication date: 2003

Host publication information
Title of host publication: SDMA 2003 and ICSF V. Vol. 2
Place of publication: Bremen
Publisher: Universität Bremen
Editors: Bauckhage, K., Fritsching, U., Uhlenwinkel, V., Ziesenis, J., Leatham, A.
ISBN (Print): 3833005718
Source: orbit
Source-ID: 305771

Bulk amorphous Mg-based alloys
Characteristics, crystallization processes and micro/nano formability of bulk amorphous alloys

Deformation characteristics of Mg$_{60}$Cu$_{30}$Y$_{10}$ alloy at temperatures near Tg

Den usædvanlige formbarhed af bulk metalglasser

Rapid solidification of martensitic stainless steel atomized droplets
Structure annealing characteristics and mechanical properties of Mg$_{80}$Cu$_{30-y}$Y$_y$Si$_{10}$ bulk amorphous alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wolff, U., Yang, B., Pryds, N., Wert, J. A.
Publication date: 2002
Peer-reviewed: No
Event: Abstract from 2002 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Source: orbit
Source-ID: 304997
Research output: Research › Conference abstract for conference – Annual report year: 2002

Undercooling in Pd$_{40}$Cu$_{30}$Ni$_{10}$P$_{20}$ melt

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Linderoth, S., Jiang, J.
Publication date: 2002
Peer-reviewed: No
Event: Abstract from 2. International conference on bulk metallic glasses (Bulk metallic glasses II), Keelung (TW), 24-28 Mar.,
Source: orbit
Source-ID: 304037
Research output: Research › Conference abstract for conference – Annual report year: 2002

A geometrical model for the prediction of the billet shape in spray forming

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pedersen, T., Hattel, J., Pryds, N.
Pages: 353-358
Publication date: 2001

Host publication information
Title of host publication: Science of metastable and nanocrystalline alloys. Structure, properties and modelling.
Proceedings
Place of publication: Roskilde
Publisher: Risø National Laboratory
ISBN (Print): 87-550-2916-7
URLs:
Amorphous magnesium alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Eldrup, M. M., Linderoth, S., Pryds, N., Pedersen, A. S., Ohnuma, M.
Pages: 163-175
Publication date: 2001

Host publication information
Title of host publication: Sammensatte materialer. Fremstilling, egenskaber, anvendelse
Place of publication: Lyngby
Publisher: DMS
Editor: Brøndsted, P.
ISBN (Print): 87-97535-30-0
Source: orbit
Source-ID: 302163
Research output: Research › Article in proceedings – Annual report year: 2001

Crystallization kinetics of Mg-Cu-Y bulk amorphous alloy

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Eldrup, M. M., Pedersen, A. S.
Pages: 377-382
Publication date: 2001

Host publication information
Title of host publication: Science of metastable and nanocrystalline alloys. Structure, properties and modelling.
Proceedings
Place of publication: Roskilde
Publisher: Risø National Laboratory
ISBN (Print): 87-550-2916-7
URLs:
Source: orbit
Source-ID: 302813
Research output: Research › Article in proceedings – Annual report year: 2001

Experimental studies on the glass formation of Mg-Cu-Sn alloy system

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Zhang, E., Pryds, N.
Pages: 449-454
Publication date: 2001

Host publication information
Title of host publication: Science of metastable and nanocrystalline alloys. Structure, properties and modelling.
Proceedings
Place of publication: Roskilde
Publisher: Risø National Laboratory
ISBN (Print): 87-550-2916-7
URLs:
On the stability and crystallisation of bulk amorphous Mg-Cu-Y-Al alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 656-659
Publication date: 2001
Peer-reviewed: Yes

Publication information
Volume: 304-306
ISSN (Print): 0921-5093
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.76 SJR 1.694 SNIP 1.943
Web of Science (2017): Impact factor 3.414
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.669 SNIP 1.913
Web of Science (2016): Impact factor 3.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.01 SJR 1.742 SNIP 1.858
Web of Science (2015): Impact factor 2.647
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.32 SJR 2.235 SNIP 2.546
Web of Science (2014): Impact factor 2.567
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.86 SJR 1.868 SNIP 2.235
Web of Science (2013): Impact factor 2.409
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.5 SJR 1.744 SNIP 2.358
Web of Science (2012): Impact factor 2.108
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.59 SJR 1.74 SNIP 2.414
Web of Science (2011): Impact factor 2.003
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.723 SNIP 2.114
Web of Science (2010): Impact factor 2.101
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.57 SNIP 1.757
Rheological properties of a $\text{Mg}_{60}\text{Cu}_{30}\text{Y}_{10}$ alloy in the supercooled liquid state

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wert, J. A., Pryds, N., Zhang, E.
Pages: 423-428
Publication date: 2001

Host publication information
Title of host publication: Science of metastable and nanocrystalline alloys. Structure, properties and modelling.
Proceedings
Place of publication: Roskilde
Publisher: Risø National Laboratory
ISBN (Print): 87-550-2916-7
URLs:
Source: orbit
Source-ID: 302814
Research output: Research - peer-review › Article in proceedings – Annual report year: 2001

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Fuel Cells and Solid State Chemistry Division
Number of pages: 500
Publication date: 2001

Publication information
The determination of dynamic and equilibrium solid/liquid transformation data for Sn-Pb using DSC

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 887-894
Publication date: 2001
Peer-reviewed: Yes

Publication information
Journal: Journal of Thermal Analysis and Calorimetry
Volume: 64
ISSN (Print): 1388-6150
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.1 SJR 0.587 SNIP 1.073
Web of Science (2017): Impact factor 2.209
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.76 SJR 0.609 SNIP 0.977
Web of Science (2016): Impact factor 1.953
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.69 SJR 0.591 SNIP 0.971
Web of Science (2015): Impact factor 1.781
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.87 SJR 0.643 SNIP 1.204
Web of Science (2014): Impact factor 2.042
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.97 SJR 0.458 SNIP 1.273
Web of Science (2013): Impact factor 2.206
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.84 SJR 0.597 SNIP 1.244
Web of Science (2012): Impact factor 1.982
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.55 SJR 0.532 SNIP 1.034
Web of Science (2011): Impact factor 1.604
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.474 SNIP 1.058
Web of Science (2010): Impact factor 1.752
BFI (2009): BFI-level 1
A new integrated numerical model for spray atomization and deposition: Comparison between numerical results and experiments

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pedersen, T., Hattel, J., Pryds, N., Pedersen, A. S., Buchholz, M., Uhlenwinkel, V.
Pages: 813-823
Publication date: 2000

Host publication information
Title of host publication: Spray deposition and melt atomization. Proceedings. Vol. 2
Place of publication: Bremen
Publisher: Universität Bremen
Editors: Bauckhage, K., Uhlenwinkel, V., Fritsching, U.
ISBN (Print): 3-88722-473-6
Source: orbit
Source-ID: 301241
Research output: Research › Article in proceedings – Annual report year: 2000

Bulk amorphous alloys: Preparation and properties of (Mg0.98Al0.02)x(Cu0.75Y0.25)(100-x)
New bulk amorphous quaternary alloys of the composition (Mg1-xAlx)(60)Cu30Y10 (x = 0 - 0.17) were recently reported by the authors and preliminary results of the influence of Al content on the ability to form a bulk amorphous phase were presented. In the present note we extend this work to look for the influence of the Mg-Al content on the glass forming ability by studying a range of compositions, (Mg0.98Al0.02)(x)(Cu0.75Y0.25)(100-x) for x = 60 - 80 at.%. As previously, the alloys were prepared by a relatively simple technique, i.e. rapid cooling of the melt in a wedge-shaped copper mould. This method provides a range of cooling rates within a single ingot during the solidification that link the slowly and rapidly cooled microstructure for each alloy composition. Hence, the maximum thickness of the amorphous part of the cast material will be a measure of the glass forming ability (GFA) of the particular alloy. X-ray diffraction (XRD) and Differential Scanning Calorimetry (DSC) have been used to investigate the structure and the various structural transitions in the alloys. One observation is that the GFA decreases with increasing content of (Mg0.98Al0.02)(x). For x > similar to 75 at.% no amorphous phase is formed. Based on these measurements a phase diagram was constructed.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 123-128
Publication date: 2000
Bulk amorphous Mg-Cu-Y alloys in the as-prepared, supercooled liquid and crystalline states

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Publication date: 2000
Peer-reviewed: No
Event: Abstract from MRS 2000 Fall meeting, Boston, MA (US), 27 Nov - 1 Dec.
Source: orbit
Source-ID: 301546
Research output: Research › Conference abstract for conference – Annual report year: 2000

Crystallography and morphology of cementite precipitates formed during rapid solidification of a ferritic stainless steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Huang, X., Pryds, N.
Pages: 4073-4082
Publication date: 2000
Peer-reviewed: Yes

Publication information
Volume: 48
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Impact factor 6.036
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Impact factor 5.301
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.22 SJR 3.417 SNIP 2.831
Web of Science (2015): Impact factor 5.058
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.16 SJR 3.885 SNIP 3.166
Web of Science (2014): Impact factor 4.465
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Numerical modelling of the spray forming process: The effect of process parameters on the deposited material

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Risø National Laboratory for Sustainable Energy
Contributors: Hattel, J. H., Pryds, N., Pedersen, T. B., Pedersen, A. S.
Pages: 803-812
On the Spray Forming Process: Numerical Modelling of Atomized and Compacted Metal

Abstract

Preparation and properties of Mg-Cu-Y-Al bulk amorphous alloys

Preparation and Properties of Mg-Cu-Y-Al bulk Amorphous Alloys

Bulk amorphous (Mg(1-gamma)Al(gamma))(60)CU(30)Y(10) alloys were prepared using a relatively simple technique of rapid cooling of the melt in a copper wedge mould. The temperature vs, time was recorded during the cooling and solidification process of the melt and compared with a spacial and temporal numerical simulation of that process. It is concluded that good thermal contact is maintained between the amorphous part of the solidified sample and the mould, while a rather poor contact develops between the crystalline part of the sample and the mould, probably due to the appearance of a narrow gap at the crystal-mould interface during crystallisation. The maximum amorphous layer thickness decreases from similar to3 mm to zero when the Al content increases in the range from 0 to about y = 10%. The evolution of the microstructure of the initially amorphous phase was examined by x-ray diffraction (XRD) and differential scanning calorimetry (DSC) for different alloy compositions and annealing temperatures. On annealing into the supercooled liquid state (441 K), specimens with no Al content remain basically amorphous while nanoparticles are formed and remain stable also at higher temperatures in specimens containing a few percent Al. The alloy with no Al crystallises apparently without the formation of nanoparticles. The critical cooling rate for the formation of an amorphous Mg(60)CU(30)Y(10) specimen was determined experimentally by a combination of DSC data and temperature vs, time measurements to be 60-150 K/s, in agreement with estimates from the literature. The Vickers hardness (Hv) of the amorphous material for y = 2% is higher (similar to 360 kg/mm(2)) than for y = 0 (similar to 290 kg/mm(2)). On crystallisation the hardness of the latter material increases to the 400 kg/mm(2) level while the hardness of the former does not change.
The effect of cooling rate on the microstructures formed during solidification of ferritic steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Huang, X.
Pages: 3155-3166
Publication date: 2000
Peer-reviewed: Yes

Publication information
Journal: Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science
Volume: 31
ISSN (Print): 1073-5623
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.08 SJR 1.093 SNIP 1.28
Web of Science (2017): Impact factor 1.887
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.91 SJR 1.206 SNIP 1.336
Web of Science (2016): Impact factor 1.874
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.78 SJR 1.267 SNIP 1.407
Web of Science (2015): Impact factor 1.749
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.06 SJR 1.659 SNIP 1.848
Web of Science (2014): Impact factor 1.73
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.9 SJR 1.513 SNIP 1.656
Web of Science (2013): Impact factor 1.73
ISI indexed (2013): ISI indexed yes
The effect of particles in different sizes on the mechanical properties of spray-formed steel composites

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Petersen, K., Pedersen, A. S., Pryds, N., Thorsen, K., List, J.
Pages: 147-160
Publication date: 2000

Host publication information
Title of host publication: Spray deposition and melt atomization. Proceedings. Vol. 1
Place of publication: Bremen
Publisher: Universität Bremen
Editors: Bauckhage, K., Uhlenwinkel, V., Fritsching, U.
ISSN (Print): 3-88722-473-6
Source: orbit
The extraction of equilibrium solid/liquid transformation data from dynamic DSC measurements

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Publication date: 2000
Peer-reviewed: No
Event: Abstract from 12th International Congress on Thermal Analysis and Calorimetry, Copenhagen, Denmark.
Source: orbit
Source-ID: 301267
Research output: Research › Conference abstract for conference – Annual report year: 2000

A quasi-stationary numerical model of atomized metal droplets. 1: Model formulation

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Hattel, J., Pryds, N., Thorborg, J., Ottosen, P.
Pages: 413-430
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Modelling and Simulation in Materials Science and Engineering
Volume: 7
ISSN (Print): 0965-0393
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.8 SJR 0.821 SNIP 0.93
Web of Science (2017): Impact factor 1.793
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.82 SJR 1.076 SNIP 1.05
Web of Science (2016): Impact factor 1.891
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.73 SJR 1.225 SNIP 1.057
Web of Science (2015): Impact factor 1.859
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.81 SJR 1.305 SNIP 1.157
Web of Science (2014): Impact factor 2.167
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.25 SJR 1.083 SNIP 1.197
Web of Science (2013): Impact factor 1.492
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.05 SJR 1.461 SNIP 1.794
Web of Science (2012): Impact factor 1.932
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
A quasi-stationary numerical model of atomized metal droplets. 2: Prediction and assessment

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Hattel, J., Thorborg, J.
Pages: 431-446
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Modelling and Simulation in Materials Science and Engineering
Volume: 7
ISSN (Print): 0965-0393
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.8 SJR 0.821 SNIP 0.93
Web of Science (2017): Impact factor 1.793
Web of Science (2017): Indexed yes
Bulk amorphous alloys: Preparation and properties of $(\text{Mg}_{0.98}\text{Al}_{0.02})_x(\text{Cu}_{0.75}\text{Y}_{0.25})_{100-x}$

General information

State: Published
Publication date: 1999
Peer-reviewed: No
Event: Abstract from International symposium on metastable, mechanically alloyed and nanocrystalline materials (ISMANAM-99), Dresden (DE), 29 Aug - 3 Sep, .
Source: orbit
Source-ID: 299277
Research output: Research › Conference abstract for conference – Annual report year: 1999

Bulk amorphous $(\text{Mg}_{0.98}\text{Al}_{0.02})_{60}\text{Cu}_{30}\text{Y}_{10}$ alloy

General information

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 889-893
Publication date: 1999
Peer-reviewed: Yes

Publication information

Journal: Scripta Materialia
Volume: 41
ISSN (Print): 1359-6462
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.19 SJR 1.923 SNIP 1.855
Web of Science (2017): Impact factor 4.163
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.884 SNIP 1.737
Web of Science (2016): Impact factor 3.747
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.54 SJR 2.259 SNIP 1.841
Web of Science (2015): Impact factor 3.305
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.55 SJR 2.65 SNIP 2.035
Web of Science (2014): Impact factor 3.224
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.19 SJR 2.323 SNIP 1.946
Web of Science (2013): Impact factor 2.968
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.01 SJR 2.292 SNIP 1.996
Web of Science (2012): Impact factor 2.821
ISI indexed (2012): ISI indexed yes
Gør metaller bedre

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Leffers, T., Pryds, N.
Pages: 10-11
Publication date: 1999
Peer-reviewed: Unknown

Publication information
Journal: Risønyt
Issue number: 4
Original language: Danish
URLs:
On the effect of Al on the formation of amorphous Mg-Al-Cu-Y alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 119-124
Publication date: 1999

Host publication information
Title of host publication: Bulk metallic glasses
Place of publication: Warrendale, PA
Publisher: Materials Research Society
Editors: Johnson, W., Liu, C., Inoue, A.
(Materials Research Society Symposium Proceedings, 554).
Source: orbit
Source-ID: 299242
Research output: Research › Article in proceedings – Annual report year: 1999

On the stability and crystallization process of bulk amorphous Mg-Cu-Y-Al alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Linderoth, S., Pryds, N., Ohnuma, M., Pedersen, A. S., Eldrup, M. M.
Publication date: 1999
Peer-reviewed: No
Event: Abstract from 10th International meeting on rapidly quenched materials, Bangalore, India.
Source: orbit
Source-ID: 299026
Research output: Research › Conference abstract for conference – Annual report year: 1999

The solidification characteristics of laser surface-remelted Fe-12Cr-nC alloys

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Juhl, T., Pedersen, A. S.
Pages: 1817-1828
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science
Volume: 30
ISSN (Print): 1073-5623
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.08 SJR 1.093 SNIP 1.28
Web of Science (2017): Impact factor 1.887
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.91 SJR 1.206 SNIP 1.336
Web of Science (2016): Impact factor 1.874
A numerical model of atomized metal droplets in the spray-forming process

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Hattel, J.
Publication date: 1998

Host publication information
Title of host publication: Proceedings
Place of publication: Lyngby
Publisher: Danmarks Tekniske Universitet, Institut for Procesteknik
Source: orbit
Source-ID: 297822
Research output: Research › Conference abstract in proceedings – Annual report year: 1998

Microstructural investigation of a rapidly solidified 12Cr-Mo-V steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Johnson, E., Linderoth, S., Pedersen, A. S.
Pages: 367-376
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science
Volume: 29
ISSN (Print): 1073-5623
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.08 SJR 1.093 SNIP 1.28
Web of Science (2017): Impact factor 1.887
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.91 SJR 1.206 SNIP 1.336
Web of Science (2016): Impact factor 1.874
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.78 SJR 1.267 SNIP 1.407
Web of Science (2015): Impact factor 1.749
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.06 SJR 1.659 SNIP 1.848
Web of Science (2014): Impact factor 1.73
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.9 SJR 1.513 SNIP 1.656
Web of Science (2013): Impact factor 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 1.76 SJR 1.426 SNIP 1.75
Numerical modelling of rapid solidification

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Hattel, J.
Publication date: 1998

Host publication Information
Title of host publication: Proceedings
Place of publication: Lyngby
Publisher: Danmarks Tekniske Universitet, Institut for Procesteknik
Source: orbit
Source-ID: 298915
Research output: Research › peer-review › Journal article – Annual report year: 1998

On the effect of Al on the formation of amorphous Mg-Al-Cu-Y alloys

General information
On the lack of dependence of extent of columnar growth on wheel speed for melt-spun 12Cr-Mo-V steel

General information
State: Published
Organisations: Department of Manufacturing Engineering, Risø National Laboratory for Sustainable Energy
Contributors: Hattel, J. H., Pryds, N.
Pages: 723-727
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Scripta Materialia
Volume: 38
Issue number: 5
ISSN (Print): 1359-6462
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.19 SJR 1.923 SNIP 1.855
Web of Science (2017): Impact factor 4.163
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.884 SNIP 1.737
Web of Science (2016): Impact factor 3.747
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.54 SJR 2.259 SNIP 1.841
Web of Science (2015): Impact factor 3.305
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.55 SJR 2.65 SNIP 2.035
Web of Science (2014): Impact factor 3.224
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.19 SJR 2.323 SNIP 1.946
Web of Science (2013): Impact factor 2.968
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.01 SJR 2.292 SNIP 1.996
Web of Science (2012): Impact factor 2.821
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.21 SJR 2.314 SNIP 2.082
Web of Science (2011): Impact factor 2.699
The relation between experiments and modeling of rapidly solidified 12Cr-Mo-V stainless steel

Solidification during melt spinning of a 12Cr-Mo-V stainless steel has been experimentally studied and numerically simulated. The resulting microstructures have been related to the unknown parameter h, i.e. the heat transfer coefficient between the substrate and the melt, by fitting the heat flow calculations and a phase selection model for a multicomponent system to the observed microstructures. Using the estimated value of the heat transfer coefficient, it was then possible to explain the observed structures in terms of growth velocities. High growth velocities (> 0.2 m s\(^{-1}\)) resulted in formation of metastable austenite as the primary phase near the chill side of the ribbon. Upon quenching to room temperature, this austenite transformed into martensite. At a distance of about 15 μm from the chill surface, the growth velocity of the solid/liquid interface decreased (< 0.2 m s\(^{-1}\)), allowing the stable ferrite phase to form as the primary phase. This approach provides a means to determine the solidification parameters and the microstructures formed in this rapid solidification process. (C) 1998 Elsevier Science S.A. All rights reserved.
The solidification structures in atomized droplets of martensitic stainless steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Pages: 217-236
Publication date: 1998

Host publication information
Title of host publication: Pulvermaterialer
Place of publication: Lyngby
Publisher: DMS
Editors: Brøndsted, P., Grønning Sørensen, K.
ISBN (Print): 87-87535-27-0
Source: orbit
Source-ID: 298942
Research output: Research › Article in proceedings – Annual report year: 1998

Analysis of the solidification during the spray deposition process

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Larsen, B.
Publication date: 1997
Peer-reviewed: No
Event: Abstract from Joint Nordic Conference in Powder Technology, Helsinki, Finland.
Source: orbit
Source-ID: 296544
Research output: Research › Conference abstract for conference – Annual report year: 1997

Numerical modelling of rapid solidification
A mathematical model of the melt spinning process has been developed based on the control-volume finite-difference method. The model avoids some of the limitations of the previous models, for example including the effect of the wheel in the heat flow calculations and the temperature dependence of the thermophysical parameters of the material. The nucleation temperature was calculated based on the heterogeneous nucleation theory.

The effect of various parameters, such as the heat transfer coefficient, the nucleation temperature and the heating and type of the wheel on the rapid solidification behaviour, for example the recalescence characteristic, was investigated. The results of the model showed that the effect of heating of the wheel is difficult to prevent even for a wheel material of high conductivity. The recalescence effect was found to be influenced by the wheel surface temperature and to decrease with increasing thermal conductivity of the wheel.
The observed increase in the wheel surface temperature suggests the importance of including the wheel in the numerical calculations, especially for a wheel made of a low-conductive material.

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Department of Manufacturing Engineering
Contributors: Pryds, N., Hattel, J. H.
Pages: 451-472
Publication date: 1997
Peer-reviewed: Yes

**Publication information**

Journal: Modelling and Simulation in Materials Science and Engineering
Volume: 5
Issue number: 5
ISSN (Print): 0965-0393
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.8 SJR 0.821 SNIP 0.93
Web of Science (2017): Impact factor 1.793
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.82 SJR 1.076 SNIP 1.05
Web of Science (2016): Impact factor 1.891
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.73 SJR 1.225 SNIP 1.057
Web of Science (2015): Impact factor 1.859
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.81 SJR 1.305 SNIP 1.157
Web of Science (2014): Impact factor 2.167
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.25 SJR 1.083 SNIP 1.197
Web of Science (2013): Impact factor 1.492
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.05 SJR 1.461 SNIP 1.794
Web of Science (2012): Impact factor 1.932
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.96 SJR 1.151 SNIP 1.362
Web of Science (2011): Impact factor 2.298
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.244 SNIP 1.307
Web of Science (2010): Impact factor 1.387
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.16 SNIP 1.165
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.263 SNIP 1.097
Planar colony of needle precipitates formed during solidification of a ferritic stainless steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N., Huang, X.
Pages: 1219-1226
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: Scripta Materialia
Volume: 36
ISSN (Print): 1359-6462
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.19 SJR 1.923 SNIP 1.855
Web of Science (2017): Impact factor 4.163
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.884 SNIP 1.737
Web of Science (2016): Impact factor 3.747
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.54 SJR 2.259 SNIP 1.841
Web of Science (2015): Impact factor 3.305
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.55 SJR 2.65 SNIP 2.035
Web of Science (2014): Impact factor 3.224
Rapid solidification of the 12% Cr steel

General information
State: Published
Organisations: Thermo Ceramics, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy
Microstructural evolution during rapid solidification of stainless steel

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Publication date: 1996
Peer-reviewed: No
Event: Abstract from Joint Nordic Conference in Powder Technology, Copenhagen, Denmark.
Source: orbit
Source-ID: 294770
Research output: Research › Conference abstract for conference – Annual report year: 1996

Microstructure of rapidly solidified Cr-Mo-v

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pryds, N.
Publication date: 1994
Peer-reviewed: No
Source: orbit
Source-ID: 291673
Research output: Research › Conference abstract for conference – Annual report year: 1994

Projects:

Fabrication and electrical properties of advanced thin film materials for resistive switching memories
Li, Y., PhD Student, Department of Energy Conversion and Storage
Pryds, N., Main Supervisor, Department of Energy Conversion and Storage
Esposito, V., Supervisor, Department of Energy Conversion and Storage
Sanna, S., Supervisor, Department of Energy Conversion and Storage
Traulsen, M. L., Supervisor, Department of Energy Conversion and Storage
Forskningsrådssnansiering
01/04/2017 → 31/03/2020
Award relations: Fabrication and electrical properties of advanced thin film materials for resistive switching memories
Project: PhD

Giant-E - Ceria Thin Films Giant Electrostrictors
Santucci, S., PhD Student, Department of Energy Conversion and Storage
Esposito, V., Main Supervisor, Department of Energy Conversion and Storage
Lubomirsky, I., Supervisor
Pryds, N., Supervisor, Department of Energy Conversion and Storage
Forskningsrådssnansiering
15/02/2017 → 14/02/2020
Award relations: Giant-E - Ceria Thin Films Giant Electrostrictors
Project: PhD
Density functional theory based modelling of materials for resistive switching memories
Pedersen, C. S., PhD Student, Department of Energy Conversion and Storage
García Lastra, J. M., Main Supervisor, Department of Energy Conversion and Storage
Pryds, N., Supervisor, Department of Energy Conversion and Storage
Vegge, T., Supervisor, Department of Energy Conversion and Storage
Forskningsrådsfinansiering
01/01/2017 → 31/12/2019
Award relations: Density functional theory based modelling of materials for resistive switching memories
Project: PhD

NICE: The fabrication and testing of two terminal memristor device - Nano Ionic Conducting Engineered materials for information application
Pryds, N., Project Manager, Department of Energy Conversion and Storage, Electrofunctional materials
Esposito, V., Project Participant, Department of Energy Conversion and Storage, Ceramic Engineering & Science
Traulsen, M. L., Project Participant, Department of Energy Conversion and Storage, Fundamental Electrochemistry
External Project ID: DFF-FTP Research project 2
01/01/2017 → 31/01/2020
Collaborators: Swiss Federal Institute of Technology Zurich
Project: Research

Fabrication and electrical properties of correlated electron systems at the interfaces of complex oxides
Gan, Y., PhD Student, Department of Energy Conversion and Storage
Chen, Y., Main Supervisor, Department of Energy Conversion and Storage
Pryds, N., Supervisor, Department of Energy Conversion and Storage
Institut stipendie (DTU)
01/10/2016 → 30/09/2019
Award relations: Fabrication and electrical properties of correlated electron systems at the interfaces of complex oxides
Project: PhD

Developing New Electrolytes Materials and Methods for the Manufacture of Nanostructured Electrolytes for Low Temperature SOFC Operating Around 400°C
Janik, K. A., PhD Student, Risø National Laboratory for Sustainable Energy
Pryds, N., Main Supervisor, Risø National Laboratory for Sustainable Energy
Esposito, V., Supervisor, Department of Energy Conversion and Storage
Kuhn, L. T., Supervisor, Risø National Laboratory for Sustainable Energy
Linderøth, S., Supervisor, Risø National Laboratory for Sustainable Energy
Holtappels, P., Examiner, Department of Energy Conversion and Storage
Amoruso, S., Examiner
Feidenhans'l, R. K., Examiner, Department of Chemistry
Feidenhans'l, R., Examiner
Institut/centerfinansieret
01/08/2007 → 28/09/2011
Award relations: Developing New Electrolytes Materials and Methods for the Manufacture of Nanostructured Electrolytes for Low Temperature SOFC Operating Around 400°C
Project: PhD

Magnetisk køling
Petersen, T. F., PhD Student, Department of Mechanical Engineering
Elmegaard, B., Main Supervisor, Department of Mechanical Engineering
Knudsen, H. H., Supervisor, Department of Mechanical Engineering
Linderøth, S., Supervisor
Pryds, N., Supervisor
Smith, A., Supervisor
Carlsen, H., Examiner, Department of Mechanical Engineering
Rowe, A., Examiner
Veje, C. T., Examiner
Risø (Løn)
01/10/2004 → 06/02/2008
Award relations: Magnetisk køling
Hurtig-størkning af rustfrit stål
Pryds, N., PhD Student
Hansen, P. N., Main Supervisor
Forskerakademiets Samfinansier
01/03/1994 → 22/05/1997
Award relations: Hurtig-størkning af rustfrit stål
Project: PhD

Electrical Properties of Correlated Electron Systems at the Interfaces of Complex Oxides
von Soosten, M., PhD Student, Department of Energy Conversion and Storage
Pryds, N., Main Supervisor, Department of Energy Conversion and Storage
Chen, Y., Supervisor, Department of Energy Conversion and Storage
Jespersen, T. S., Supervisor
Institut stipendie (DTU)
01/12/2015 → 30/06/2019
Award relations: Electrical Properties of Correlated Electron Systems at the Interfaces of Complex Oxides
Project: PhD

The role of contact resistance in thermoelectric module
Malik, S. A., PhD Student, Department of Energy Conversion and Storage
Van Nong, N., Main Supervisor, Department of Energy Conversion and Storage
Stamate, E., Supervisor, Department of Energy Conversion and Storage
Kaiser, A., Examiner, Department of Energy Conversion and Storage
Pryds, N., Examiner, Department of Energy Conversion and Storage
Rezaniakolaei, A., Examiner
Eklund, P., Examiner
Rezaniakolaei, A., Examiner
Forskningsrådsfinansiering
15/02/2015 → 12/11/2018
Award relations: The role of contact resistance in thermoelectric module
Project: PhD

Flavour Release from Model Systems - In Vitro and In Vivo Instrumental Measurements
Dinesen, A. R., PhD Student, Department of Physics
Mørup, S., Main Supervisor, Department of Physics
Linderoth, S., Supervisor
Pryds, N., Supervisor
Jacobsen, C. S., Examiner, Department of Physics
Pankhurst, Q. A., Examiner
Rasmussen, F. B., Examiner
Forskerakademiets Samfinansier
01/03/2000 → 28/05/2003
Award relations: Flavour Release from Model Systems - In Vitro and In Vivo Instrumental Measurements
Project: PhD

Modelling of residual stresses in spray formed structures
Pedersen, T. B., PhD Student, Department of Management Engineering
Hattel, J. H., Main Supervisor, Department of Management Engineering
Pryds, N., Supervisor
Hansen, P. N., Examiner
Doherty, R. D., Examiner
Fritsching, U. W., Examiner
Risø (Løn)
01/05/1999 → 04/04/2003
Award relations: Modelling of residual stresses in spray formed structures
Project: PhD

Relationship between microstructural defects and performance in 2nd generation HTS tapes
Li, X., PhD Student, Risø National Laboratory for Sustainable Energy
Development and processing of p-type oxide thermoelectric materials
Wu, N., PhD Student, Department of Energy Conversion and Storage
Linderoth, S., Main Supervisor, Department of Energy Conversion and Storage
Nong, N. V., Supervisor
Pryds, N., Supervisor, Risø National Laboratory for Sustainable Energy
Bahl, C., Examiner, Department of Physics
Balke, B., Examiner
Eklund, P., Examiner
Forskningsrådsfinansiering
01/08/2011 → 26/11/2014
Award relations: Development and processing of p-type oxide thermoelectric materials
Project: PhD

Modeling of shape instabilities occurring during sintering
Tadesse Molla, T., PhD Student, Department of Energy Conversion and Storage
Frandsen, H. L., Main Supervisor, Department of Energy Conversion and Storage
Bjørk, R., Supervisor, Department of Energy Conversion and Storage
Pryds, N., Supervisor, Department of Energy Conversion and Storage
Hattel, J. H., Examiner
Bordia, R. K., Examiner
Raether, F., Examiner
Forskningsrådsfinansiering
15/07/2011 → 30/09/2014
Award relations: Modeling of shape instabilities occurring during sintering
Project: PhD

Development and processing of n-type oxide thermoelectric materials
Han, L., PhD Student, Department of Energy Conversion and Storage
Linderoth, S., Main Supervisor, Department of Energy Conversion and Storage
Nong, N. V., Supervisor
Pryds, N., Supervisor, Department of Energy Conversion and Storage
Kaiser, A., Examiner, Department of Energy Conversion and Storage
Palmqvist, A., Examiner
Weidenkaff, A., Examiner
Forskningsrådsfinansiering
01/07/2011 → 30/09/2014
Award relations: Development and processing of n-type oxide thermoelectric materials
Project: PhD

Development of functionally graded thermoelectric materials based on optimal average figure-of-merit
Le, T. H., PhD Student, Risø National Laboratory for Sustainable Energy
Pryds, N., Main Supervisor, Risø National Laboratory for Sustainable Energy
Kuhn, L. T., Examiner, Risø National Laboratory for Sustainable Energy
Gelbstein, Y., Examiner
Rosendahl, L., Examiner
Gelbstein, Y., Examiner
Rosendahl, L., Examiner
Forskningsrådsfinansiering
01/06/2011 → 26/11/2014
Award relations: Development of functionally graded thermoelectric materials based on optimal average figure-of-merit
Project: PhD
Numerical modelling of tape casting of functionally graded ceramic materials
Jabbaribehnam, M., PhD Student, Department of Mechanical Engineering
Hattel, J. H., Main Supervisor, Department of Mechanical Engineering
Pryds, N., Supervisor
Frandsen, H. L., Examiner
Mitsoulis, E., Examiner
Tok, A., Examiner
Forskningsrådsfinansiering
01/02/2011 → 29/09/2014
Award relations: Numerical modelling of tape casting of functionally graded ceramic materials
Project: PhD

Numerical modelling of extrusion of functionally graded ceramic materials
Comminal, R. B., PhD Student, Department of Mechanical Engineering
Hattel, J. H., Main Supervisor, Department of Mechanical Engineering
Pryds, N., Supervisor, Risø National Laboratory for Sustainable Energy
Spangenberg, J., Supervisor, Department of Mechanical Engineering
Walther, J. H., Examiner, Department of Mechanical Engineering
Alves, M. A. M., Examiner
Kupferman, R., Examiner
Alves, M. A. M., Examiner
Kupferman, R., Examiner
Forskningsrådsfinansiering
01/01/2011 → 24/08/2015
Award relations: Numerical modelling of extrusion of functionally graded ceramic materials
Project: PhD

Magnetocaloric regenerator design
Jensen, J. B., PhD Student, Risø National Laboratory for Sustainable Energy
Pryds, N., Main Supervisor, Risø National Laboratory for Sustainable Energy
Bahl, C., Supervisor, Risø National Laboratory for Sustainable Energy
Elmegaard, B., Supervisor
Carlsen, H., Examiner
Kitanovski, A., Examiner
Veje, C. T., Examiner
Forskningsrådsfinansiering
15/03/2008 → 19/10/2011
Award relations: Magnetocaloric regenerator design
Project: PhD

Modeling of Active Magnetic Regenerators for Magnetic Refrigeration at Room Temperature
Nielsen, K. K., PhD Student, Department of Energy Conversion and Storage
Hattel, J. H., Main Supervisor, Department of Management Engineering
Bahl, C., Supervisor, Department of Physics
Pryds, N., Supervisor, Risø National Laboratory for Sustainable Energy
Smith, A., Supervisor, Risø National Laboratory for Sustainable Energy
Veje, C. T., Examiner
Gutfleisch, O., Examiner
Sandeman, K. G., Examiner
Forskningsrådsfinansiering
01/09/2007 → 21/12/2010
Award relations: Modeling of Active Magnetic Regenerators for Magnetic Refrigeration at Room Temperature
Project: PhD

Modeling and development of permanent magnets for magnetic refrigeration at room temperature
Bjørk, R., PhD Student, Department of Energy Conversion and Storage
Pryds, N., Main Supervisor, Risø National Laboratory for Sustainable Energy
Bahl, C., Supervisor, Department of Physics
Smith, A., Supervisor, Risø National Laboratory for Sustainable Energy
Hendriksen, P. V., Examiner, Risø National Laboratory for Sustainable Energy
Coey, J. M. D., Examiner
Rowe, A., Examiner
Forskningsrådsfinansiering
01/04/2007 → 22/09/2010
Award relations: Modeling and development of permanent magnets for magnetic refrigeration at room temperature
Project: PhD

Modelling of material flow in termomekaniske materialprocesser
Gjesing, R., PhD Student
Hattel, J. H., Main Supervisor, Department of Mechanical Engineering
Hansen, P. N., Examiner
Fritsching, U. W., Examiner
Pryds, N., Examiner
DTU-lønnet stipendie
15/11/2003 → 07/03/2008
Award relations: Modellering af materialeflow i termomekaniske materiaalprocesser
Project: PhD

Exploring Electronic Properties in All-oxide Heterostructures
Christensen, D. V., PhD Student, Department of Energy Conversion and Storage
Pryds, N., Main Supervisor, Department of Energy Conversion and Storage
Chen, Y., Supervisor, Department of Energy Conversion and Storage
Smith, A., Supervisor, Department of Energy Conversion and Storage
Nygaard, J., Examiner
Eom, C., Examiner, Department of Energy Conversion and Storage
Granzio, F. M., Examiner
Nygaard, J., Examiner
Granzio, F. M., Examiner
Institut stipendie (DTU) Samf.
01/07/2013 → 13/11/2017
Award relations: Exploring Electronic Properties in All-oxide Heterostructures
Project: PhD

Quantum and field effects of oxide heterostructures
Trier, F., PhD Student, Department of Energy Conversion and Storage
Pryds, N., Main Supervisor, Department of Energy Conversion and Storage
Chen, Y., Supervisor, Department of Energy Conversion and Storage
Jespersen, T. S., Supervisor
Thygesen, K. S., Examiner
Gabay, M., Examiner
Granzio, F. M., Examiner
Institut/centerfinansieret
01/03/2013 → 30/09/2016
Award relations: Quantum and field effects of oxide heterostructures
Project: PhD

Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery
Pham, H. N., PhD Student, Electrofunctional materials
Pryds, N., Main Supervisor, Department of Energy Conversion and Storage
Linderoth, S., Supervisor, Department of Energy Conversion and Storage
Nong, N. V., Supervisor
Ramousse, S., Examiner, Department of Energy Conversion and Storage
Eklund, P., Examiner
Roch, A., Examiner
Eklund, P., Examiner
Institut, samfinansiering
01/02/2012 → 02/12/2015
Award relations: Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery
Project: PhD

Thin-film deposition and characterization of new solar cell materials
Cazzaniga, A. C., PhD Student, Department of Photonics Engineering
Schou, J., Main Supervisor, Department of Photonics Engineering
Design of functional nanomaterials

To establish a research collaboration encompassing all steps in the development of new functional nanomaterials: design, synthesis, characterization, and testing. The common aim of the proposal is the development of rational design strategies for nano-structured materials.

Nørskov, J. K., Project Manager, Department of Physics
Jacobsen, K. W., Project Participant, Department of Physics
Chorkendorff, I., Project Participant, Department of Physics
Nielsen, J. H., Project Participant, Department of Physics
Horch, S., Project Participant, Department of Physics
Schiøtz, J., Project Participant, Department of Physics
Quaade, U., Project Participant, Department of Physics
Christensen, C. H., Project Participant, Department of Chemistry
Ulstrup, J., Project Participant, Department of Chemistry
Johannessen, T., Project Participant, Department of Chemical and Biochemical Engineering, Administration
Bægild, P., Project Participant, Department of Micro- and Nanotechnology
Pedersen, A. S., Project Participant, Risø National Laboratory for Sustainable Energy
Linderoth, S., Project Participant, Risø National Laboratory for Sustainable Energy
Mogensen, M., Project Participant, Risø National Laboratory for Sustainable Energy
Vegge, T., Project Participant, Risø National Laboratory for Sustainable Energy
Pryds, N., Project Participant, Risø National Laboratory for Sustainable Energy
Henriksen, P. V., Project Participant
Kuhn, L. T., Project Participant, Risø National Laboratory for Sustainable Energy

Project ID: 20195

Forskningsrådene - Andre: DKK9,290,000.00
01/01/2005 → 31/12/2008

Award relations: Design of functional nanomaterials

Project: Research

Activities:

Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency

Period: 26 Jun 2017 → 30 Jun 2017
Jørgen Schou (Guest lecturer)
Andrea Carlo Cazzaniga (Other)
Stela Canulescu (Other)
Andrea Crovetto (Other)
Rebecca Bolt Ettlinger (Other)
Nini Pryds (Guest lecturer)
Ole Hansen (Other)
Chang Yan (Other)
Kaiwen Sun (Other)
Xiaojing Hao (Other)

Department of Photonics Engineering
Optical Microsensors and Micromaterials
Department of Physics
Experimental Surface and Nanomaterials Physics
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency

EMRS Spring meeting 2017
Period: 23 May 2017
Jørgen Schou (Participant)
Andrea Carlo Cazzaniga (Participant)
Stela Canulescu (Organizer)
Rebecca Bolt Ettlinger (Participant)
Nini Pryds (Participant)
Ole Hansen (Organizer)
Andrea Crovetto (Organizer)
Chang Yan (Participant)
Kaiwen Sun (Participant)
Xiaojing Hao (Participant)

Description
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% efficiency

Degree of recognition: International

Abstract Earth-abundant CZTS

Related event
EMRS Spring meeting 2017
22/05/2017 → 26/05/2017
Strasbourg, France
Activity: Attending an event › Participating in or organising a conference
Materials Research Society Spring Meeting 2017
Period: 17 Apr 2017 → 21 Apr 2017
Jørgen Schou (Organizer)
Andrea Carlo Cazzaniga (Participant)
Andrea Crovetto (Participant)
Rebecca Bolt Ettlinger (Participant)
Sara Lena Josefin Engberg (Participant)
Stela Canulescu (Participant)
Nini Pryds (Participant)
Ole Hansen (Participant)
Chang Yan (Participant)
Kaiwen Sun (Participant)
Xiaojing Hao (Participant)
Department of Photonics Engineering
Photovoltaic Materials and Systems
Department of Physics
Experimental Surface and Nanomaterials Physics
Optical Microsensors and Micromaterials
Technical University of Denmark
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Micro- and Nanotechnology
Silicon Microtechnology

Description
Pulsed laser deposition (PLD) of a CZTS-absorber for thin solar cells with up to 5.2% efficiency
Degree of recognition: International
Documents:
MRS 2017_poster_JS_2

Related event
Materials Research Society Spring Meeting 2017
17/04/2017 → 21/04/2017
Phoenix, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Design, Modeling and Optimization of Thermoelectrical Power Generation Devices
Period: 10 Dec 2012
Nini Pryds (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
PHD Examiner
Activity: Examinations and supervision › External examination

2012 MRS Fall Meeting & Exhibit
Nini Pryds (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Oxide Thin Films for Renewable Energy Applications

Related event

2012 MRS Fall Meeting & Exhibit
25/11/2012 → 30/11/2012
Boston, MA, United States
Activity: Attending an event › Participating in or organising a conference

Oxides in Environment-friendly Technologies
Period: 3 Nov 2012
Nini Pryds (Invited speaker)
Electrofunctional materials
Department of Energy Conversion and Storage
Description
Invited speaker at our G-COE International Symposium, Japan
http://ncrs.cm.kyushu-u.ac.jp/ncrs2/home.html

Oxides in Environment-friendly Technologies

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Reconstructions at complex oxide Interfaces
Period: 23 Mar 2012
Nini Pryds (External examiner)
Electrofunctional materials
Department of Energy Conversion and Storage
Description
Members of the examining committee.
Activity: Examinations and supervision › External examination

Thermoelectric Oxide Materials for Heat Recovery
Period: 9 Feb 2012
Nini Pryds (Lecturer)
Electrofunctional materials
Department of Energy Conversion and Storage
Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations