



20th International Conference on

Advanced Energy Materials and Research

August 13-14, 2018 | Dublin, Ireland

Scientific Tracks & Abstracts Day 1

Advanced Energy Materials 2018

SESSIONS

Advanced Energy Materials

Chair: Xiaodong Li, University of Virginia, USA

Chair: Klaus D. Becker, TU Braunschweig, Germany

SESSION INTRODUCTION

- Title:** ^{57}Fe Mössbauer in situ study into oxygen vacancy disorder of BSCF, $\text{Ba}_{0.5}\text{Sr}_{0.5}(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$
Klaus D. Becker, TU Braunschweig, Germany
- Title:** Comparison of the thermophysical properties of eutectic with peritectic compounds for thermal energy storage at high temperatures
Fouzia Achchaq, Université de Bordeaux, France
- Title:** The role of atomic bond strengths and structural disorder in MXene materials for rechargeable ion-batteries
Wojciech Olszewski, University of Bialystok, Poland
- Title:** Laser processing of thermoelectric oxides
Nuno Ferreira, Universidade de Aveiro, Portugal
- Title:** Porous materials in heat storage and reallocation applications
Natasa Zabukovec Logar, National Institute of Chemistry and University of Nova Gorica, Slovenia
- Title:** Production and characterization of electroactive nickel oxides on nickel foam and self-standing nickel nanowires by anodic oxidation in molten salt for supercapacitor electrodes
Mustafa Urgan, Istanbul Technical University, Turkey
- Title:** Materials for thermochemical energy storage: Experimental investigation of cycling stability
Marie Gollsch, German Aerospace Center, Germany

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⁵⁷Fe Mössbauer in situ study into oxygen vacancy disorder of BSCF, $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$

Klaus D Becker¹, Piotr Gaczyński¹, Anja Harpf², Juergen Boer², Robert Kircheisen² and Ralf Kriegel²¹Braunschweig University of Technology, Germany²Fraunhofer IKTS, Germany

Although air is usually used for fuel combustion, it is well known that oxygen enrichment of combustion air enhances the combustion efficiency. Cryogenic oxygen separation is well established for oxygen production at large scale but its costs are relatively high compared to the economic benefit caused by an improved combustion efficiency. Therefore, the development of alternative oxygen separation processes is still an issue. One of the most promising ceramic materials for oxygen separation membranes is the mixed ionic electronic conducting $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$ (BSCF) with its extremely high oxygen vacancy concentration. For 900°C, for example, a value of $\delta = 0.8$ has been reported at an oxygen partial pressure of 10^{-3} bar [1,2]. We report on ⁵⁷Fe Mössbauer in situ studies of the mixed ionic electronic conducting (MIEC) oxide functional materials $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$, BSCF, conducted between room temperature and 1000°C in atmospheres of variable oxygen content in order to obtain insight into local coordination and valence of iron at working conditions and into the distribution of oxygen vacancies on their different sites. The magnetically-split room-temperature Mössbauer spectra of BSCF reveal the presence of two inequivalent iron species [3]. Evaluation of signal intensities confirms results from theoretical computations on vacancy formation in BSCF which indicate that formation energies of the various types of oxygen vacancies differ by the order of 0.1 eV only [4,5]. The analysis also shows that the distribution of vacancies is far from random [3]. In the paramagnetic high-temperature phase ($T \geq 315^\circ\text{C}$), the quadrupole-split signals demonstrate that local symmetry at iron sites is lower than cubic. At 700, 850, and 1000°C, Mössbauer centre shifts as well as quadrupole splittings are discussed in respect to stoichiometry-related changes in valence and local coordination of the iron probes.

Recent Publications

1. Yaremchenko AA, Khalyavin DD, Patrakeev MV (2017) Uncertainty of oxygen content in highly nonstoichiometric oxides from neutron diffraction data: example of perovskite-type $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$. *J. Mater. Chem. A*. 5:3456-3463
2. Tomkiewicz AC, Tamimi MA, Huq A, McIntosh S (2013) Evidence for the low oxygen stoichiometry of cubic $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.5}\text{Fe}_{0.5}\text{O}_{3-\delta}$ from in-situ neutron diffraction. *Solid State Ionics* 253:27-31
3. Gaczynski P, Harpf A, Boer J, Kircheisen R, Kriegel R, Becker K-D (2018) ⁵⁷Fe Mössbauer study into oxygen vacancy disorder of $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})\text{O}_{3-\delta}$. *Solid State Ionics* 316C:59-65
4. Kotomin EA, Mastrikov YA, Kuklja MM, Merkle R, Roytburd A, Maier J (2011) First principles calculation of oxygen vacancy formation and migration in mixed conducting $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{1-y}\text{Fe}_y)\text{O}_{3-\delta}$ perovskites. *Solid State Ionics* 188:1-5
5. Mastrikov YA, Kuklja MM, Kotomin EA, Maier J (2010) First-principles modelling of complex perovskite $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{1-y}\text{Fe}_y)\text{O}_{3-\delta}$ for oxide fuel cell and gas separation membrane applications. *Energy Environ. Sci.* 3:1544-1550.

Biography

Klaus D. Becker studied Physics at the University of Göttingen, Germany, where he received his PhD in Physical Chemistry in 1972. Subsequently, he held positions at the University of Bochum and later on at the University of Hannover. In 1995, he was appointed Professor of Physical Chemistry at Braunschweig Institute of Technology, Braunschweig, Germany. His research activities in physical chemistry of solids put particular emphasis on in-situ solid state spectroscopies applied to defects and diffusion and to the microdynamics and reaction kinetics of solids.

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Comparison of the thermophysical properties of eutectic with peritectic compounds for thermal energy storage at high temperaturesFouzia Achchaq¹, Marie Duquesne², Elena Palomo del Barrio³, Stefania Doppiu³, Eric Lebraud⁴ and Philippe Legros⁵¹Université de Bordeaux - CNRS, France²Bordeaux INP - CNRS, France³CIC EnergiGUNE, Spain⁴ICMCB - CNRS, France⁵PLACAMAT - CNRS, France

The conventional resources depletion (coal, gas, oil) and the climate change lead to the need for innovation, requiring the use of renewable energy and appropriate storage technologies. This trend involves the development of effective, reliable and cost-effective energy storage units. Our work focus on advanced energy materials for ultra-compact thermal energy storage at high temperatures (300-600°C). Thus a theoretical study, based on both literature [1-3] and FactSage 7.0[®] software, is performed to compare the stoichiometric peritectic compounds with pure and eutectic ones currently considered (molten salts, metal alloys...). The objective is to know if the peritectics can surpass the performances of these latter. The theoretical results show that the stoichiometric peritectic compounds can provide, at constant temperature and ambient pressure, a potential energy density much higher than pure and eutectic materials. This is due to their capacity to combine all advantages provided by sensible, latent and thermochemical processes. No cutting-edge technology is required to be developed for using them, contrary to the thermochemical heat storage materials [4]. Moreover, we can envision also to use the peritectic compounds in cascade ways enabling hence a consideration of very wide ranges of temperature and energy density, making them applicable to a wider pan of applications. These encouraging results fully justify the choice of stoichiometric peritectic compounds. Now, several experimental attempts are launched to determine the appropriate methods and protocols to synthesize them. To date, our work leads to the successful synthesis of the peritectic compound based on LiOH-LiBr system.

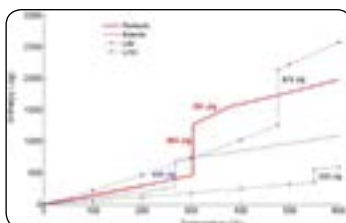


Figure 1: Example of the theoretical enthalpy evolution with temperature of four compositions of the LiOH/LiBr system: LiOH and LiBr, eutectic and peritectic mixtures.

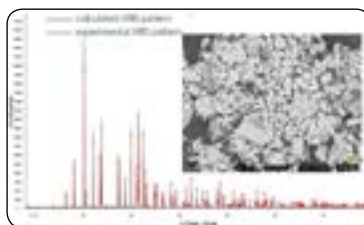


Figure 2: Calculated and experimental XRD patterns obtained for the peritectic compound based on LiOH-LiBr system.

Recent Publications

1. Kenisarin M.M (2010) High-Temperature phase change materials for thermal energy storage. *Renewable and Sustainable Energy Reviews* 27:724-37.
2. Wei G, Wang G, Xu C, Ju X, Xing L, Du X, Yang Y (2018) Selection principles and thermophysical properties of high

temperature phase change materials for thermal energy storage: A review. Renewable and Sustainable Energy Reviews 81:1771-86.

3. Reed S, Sugo H, Kisi E (2018) High temperature thermal storage materials with high energy density and conductivity. Solar Energy 163:307-14.
4. Achchaq F, Palomo del Barrio E (2017) A proposition of peritectic structures as candidates for thermal energy storage. Energy Procedia 139:346-51.

Biography

Fouzia Achchaq is Associated Professor at the University of Bordeaux and Researcher at TREFLE Department (Fluids & Transfers) of the I2M Institute and a member of TESLab (Thermal Energy Storage Laboratory), I2M/Abengoa Joint Research Unit. She has expertise in thermal energy storage materials used at high temperatures and contributes to an ANR Project Pc2TES (National Project, 2017-2020).

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Notes:

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The role of atomic bond strengths and structural disorder in MXene materials for rechargeable ion-batteries

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Ion batteries are a key technology and play a dominant role in today's world. Extensive research efforts have been dedicated to exploring and developing new cathode materials with higher capacities and lifetimes. Recently, a new family of transition metal carbides and carbonitrides called "MXene" has been synthesized with a layered hexagonal structure and $M_{n+1}AX_n$ chemistry, where M is an early transition metal, A is an A-group element (mostly groups 13 and 14), X is carbon or nitrogen, and $n=1, 2, \text{ or } 3$. MXenes have been found to be promising electrode materials, with capacities close to that of commercially available batteries and an excellent capability to handle high cycling rates. However, studies of correlation of their structural stability and functional properties could help to expand further their performances. To address this issue we have performed temperature dependent extended X-ray absorption fine structure (EXAFS) measurements at the Ti K-edge on representative members of the MXene family. Temperature dependent measurements permit to have direct access to the local force constant between the atomic pairs and correlate this information with the battery capacity and ions diffusion rate. Presented results address fundamental structural aspects that define the functional properties of electrode materials for ion batteries.

Recent Publications

1. Olszewski W, Isturiz I, Marini C, Avila M, Okubo M, Li H, Zhou H, Mizokawa T, Saini N L and Simonelli L (2018) Effects of nanostructuring on the bond strength and disorder in V_2O_5 cathode material for rechargeable ion-batteries, physical chemistry. *Chemical Physics* 20:15288-15292.
2. Simonelli L, Paris E, Wakita T, Marini C, Terashima K, Miao X, Olszewski W, Ramanan N, Heinis D, Kubozono Y, Yokoya T, Saini N L (2017) Effect of molecular intercalation on the local structure of superconducting $Nax(NH_3)_yMoSe_2$ system, *Journal of Physics and Chemistry of Solids* 111: 70-74.
3. Broux T, Bamine T, Fauth F, Simonelli L, Olszewski W, Marini C, Ménétrier M, Carlier D, Masquelier C, Croguennec L (2016) Strong impact of the oxygen content in $Na_3V_2(PO_4)_2F_{3-y}O_y$ ($0 \leq y \leq 0.5$) on its structural and electrochemical properties, *Chem. Mater.* 28: 7683–7692.
4. Olszewski W, Avila Perez M, Marini C, Paris E, Wang X, Iwao T, Masashi Y, Atsuo M, Takashi S, Saini N, Simonelli L (2016) Temperature Dependent Local Structure of $NaxCoO_2$ Cathode Material for Rechargeable Sodium-ion Batteries, *Journal of Physical Chemistry C* 120: 4227-4232.
5. Paris E, Simonelli L, Wakita T, Marini C, Lee J-H, Olszewski W, Terashima K, Kakuto T, Nishimoto N, Kimura T, Kudo K, Kambe T, Nohara M, Yokoya T, Saini N (2016) Temperature dependent local atomic displacements in ammonia intercalated iron selenide superconductor, *Scientific Reports* 6: 27646.

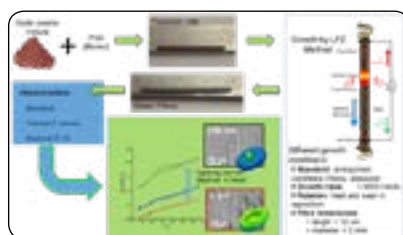
Biography

Wojciech Olszewski is a Post-Doctoral Research Associate at the ALBA Synchrotron Light Facility. He studies energy materials, and the current research direction is the investigation of the structural stability, local atomic displacements and the force constants during the diffusion process for finding a realistic correlation between the local structure and functional properties of cathode materials.

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Laser processing of thermoelectric oxidesN M Ferreira¹, M A Madre², A Sotelo², A V Kovalevsky¹ and F M Costa¹¹Universidade de Aveiro, Portugal²ICMA, CSIC-Universidad de Zaragoza, Spain

Ceramic oxides are very promising materials for thermoelectric devices, as they exhibit high Seebeck coefficient and could present relatively low electrical resistivity, as well as high chemical stability at high temperatures. Several oxides exhibit anisotropic thermoelectric properties linked to their layered structures. Therefore, texturing methods developing a preferential grain orientation, like the directional growth from the melt, are suitable to enhance the relevant physical properties. These methods have already shown their applicability to this kind of compounds and also in high T_c superconductor materials, namely, through the use of laser floating zone (LFZ) technique. The LFZ process has demonstrated its suitability for the Co-oxide based thermoelectric materials, processed in the last years in our laboratories. In this work, some examples of the versatility and usefulness of the LFZ technique are shown. The LFZ technique allows obtaining very dense, homogeneous and well textured thermoelectric composites. The results put in evidence an improvement due to electrically assisted laser floating zone on the thermoelectric performances when compared with materials processed by LFZ and by conventional techniques.

**Recent Publications**

1. A V Kovalevsky, A Myriam, S Populoh, S Patrício, N M Ferreira, S Mikhalev, D Fagg, A Weidenkaff and J R Frade (2016) Designing strontium titanate-based thermo electrics: An insight into defect chemistry mechanisms. *Journal of Materials Chemistry A* 5:3909-3922.
2. A Sotelo, F M Costa, N M Ferreira, A Kovalevsky, M C Ferro, V S Amaral, J S Amaral, S Rasekh, M A Torres, M A Madre and J C Diez (2016) Tailoring $\text{Ca}_3\text{Co}_4\text{O}_9$ microstructure and performances using a transient liquid phase sintering additive. *Journal of the European Ceramic Society* 36(4):1025-1032.
3. M A Madre, F M Costa, N M Ferreira, S I R Costa, S Rasekh, M A Torres, J C Diez, V S Amaral, J S Amaral and A Sotelo (2016) High thermoelectric performance in $\text{Bi}_{2-x}\text{Pb}_x\text{Ba}_2\text{CO}_2\text{O}_x$ promoted by directional growth and annealing. *Journal of the European Ceramic Society* 36(1):67-74.
4. Rasekh, F M Costa, N M Ferreira, M A Torres, M A Madre, J C Diez and A Sotelo (2015) Use of laser technology to produce high thermoelectric performances in $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_x$. *Materials and Design* 75:143-148.
5. F M Costa, N M Ferreira, S Rasekh, A J S Fernandes, M A Torres, M A Madre, J C Diez and A Sotelo (2015) Very large superconducting currents induced by growth tailoring. *Crystal Growth and Design* 15(5):2094-2101.

Biography

N M Ferreira is a PhD in Physics Engineering (2014), currently is a Post-Doc Researcher at i3N, Physics Department and CICECO, Department of Materials and Ceramic Engineering at University of Aveiro, Portugal. He participated as a collaborator and research fellow in several R&D projects on material science. He is an experienced researcher in study and development of ceramics-based materials, prepared through conventional methods (melting, solid stated), with particular focus on laser processing (crystal growth – LFZ and surface sintering). Present sample characterization skills include various techniques such as, electrical conductivity and magnetic properties of various oxide materials. Current focus materials: thermoelectrics, ferroelectrics and glass matrices doped with transition metals and rare earth for energy storage and conversion applications. Main expertise is related to structural, magnetic and electrical properties of materials prepared by laser processing.

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Porous materials in heat storage and reallocation applications**Natasa Zabukovec Logar**

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Thermal energy storage is recognized as one of the crucial technologies for enabling more efficient use of fossil fuels and renewable energies by providing the supply-demand balance. Thermochemical heat storage (TCS), which utilise the reversible chemical and physical sorption of gases, mostly water vapour, in solids, is currently considered as the only storage concept with a potential for long-term, also seasonal, heat storage of high enough storage density to be also economically attractive. Under the influence of a heat supply in TCS, water is desorbed from the material, which is then stored separately (an endothermic phenomenon referred to as the charging or activation of material). When water vapour and sorbent are put into contact, there is a heat release (an exothermic phenomenon referred to as a material's discharge or deactivation). The TCS has a potential to enable an extensive use of a solar thermal energy and residual heat from industry, thus leading to a low carbon energy society. Over the last decade, a lot of attention has been devoted to the development of porous adsorbents, like zeolites, microporous alumino phosphates and metal-organic framework materials for water-adsorption-based thermal energy storage and heat transformations. A good sorption-based energy-storage material should fulfil the following requirements: (i) it should exhibit high water uptake at low relative humidity, (ii) it should be easily regenerated at low temperature, and (iii) it should be highly hydrothermally stable and should enable good cycling (adsorption/desorption) performance. Recently, we have focused on the studies of microporous alumino phosphates, which show remarkable water uptake characteristics, considering the water sorption capacity, as well as superior water uptake regime and thermal stability. The studies of structure-property relationship included diffraction, spectroscopic, calorimetric and computational approaches and enabled the materials optimization. One of the alumino phosphates, AlPO_4 -LTA, outperforms all other porous materials tested so far. It exhibits superior energy-storage capacity (495 kWh m^{-3}) and shows remarkable cycling stability; after 40 cycles of adsorption/desorption its capacity drops by less than 1 wt%. Desorption temperature for this material, is lower from desorption temperatures of other tested materials by 10-15°C. This, for example, implies that regeneration of the material in a solar-energy-storage system should be easily achieved using most common types of solar collectors, e.g. flat plate collectors, even in regions without extended periods of intense solar irradiation.

**Recent Publications**

1. A Krajnc et al. (2017) Superior performance of microporous alumino phosphate with LTA topology in solar-energy storage and heat reallocation. *Advanced Energy Materials* 7(11):1601815.
2. Mazaj et al. (2017) Confined crystallization of HKUST-1 metal-organic framework within mesostructured silica with enhanced structural resistance towards water. *Journals of Materials Chemistry A* 5:22305-22315.
3. Mazaj et al. (2017) A facile strategy towards highly accessible and hydrostable MOF-phase within the hybrid poly HIPes

through in-situ metal-oxide recrystallization. *Journals of Materials Chemistry A* 5:1967-1971.

4. Krajnc et al. (2015) A simple NMR-based method for studying the spatial distribution of linkers within mixed-linker metal-organic frameworks. *Angewandte Chemie* 54(36):10535–10538.
5. Ristic et al (2012) The performance of small-pore microporous alumino phosphates in low-temperature solar energy storage: the structure-property relationship. *Advanced Functional Materials* 22(9):1952-1957.

Biography

Nataša Zabukovec Logar is a Head of the Department of Inorganic Chemistry and Technology at the National Institute of Chemistry in Ljubljana and Full Professor of Chemistry at the University of Nova Gorica. She obtained her PhD from University of Ljubljana in 1998. In 1995 and 1996 she was a visiting student at the University of Manchester, UK and in 2014, a visiting researcher at the Center for applied energy research in Munich, Germany. She has more than 20 years of experience in the research in the field of porous materials for energy and environmental applications. Her research emphases are development of new materials for gas and heat storage, and studies of metal sorption on porous solids for their use in wastewater and drinking water treatment. She is a treasurer of European Federation of Zeolite Associations and a member of the Synthesis Commission of the International Zeolite Association.

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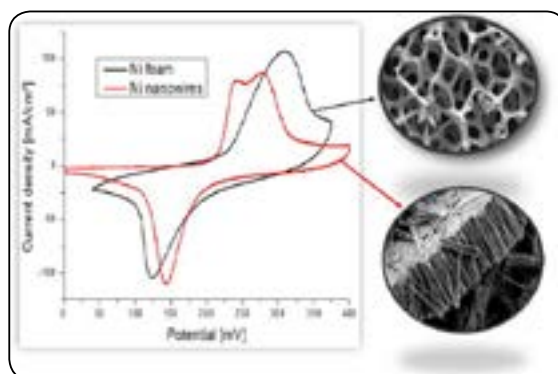
Production and characterization of electroactive nickel oxides on nickel foam and self-standing nickel nanowires by anodic oxidation in molten salt for supercapacitor electrodesMustafa Ürgen¹, Burcak Avci¹, Salvatore Pane², Bumjin Jang² and Fajer Mushtaq²¹Istanbul Technical University, Turkey²ETH-Zürich, Switzerland

Statement of the Problem: Nickel oxides, hydroxides and oxy hydroxides are promising materials for supercapacitor applications due to their high specific capacity. While indirect production of these nickel based materials is achieved either by chemical or electrochemical routes, the direct production on nickel metal itself has proved challenging. However, direct production should be investigated because it would facilitate the electron transfer required for redox reactions on the electrode surface, leading to much higher capacitances than those of the electrodes prepared with mixing nickel based materials and polymer blends.

Methodology & Theoretical Orientation: In the previous studies conducted in our group, we adapted molten salt electrolysis in KOH to directly synthesize nickel oxides on Ni foam. Here, we use the optimum parameters to synthesize nickel oxides on Ni foam and self-standing nickel nanowires (Ni NW) produced by electro deposition in AAO templates. These structures are characterized by XRD, SEM and Raman spectroscopy. The structure and the capacitance behavior are determined by cyclic voltammetry (CV) and chronopotentiometry in 6 M KOH solution.

Findings: After anodic oxidation, Ni foam and Ni NWs exhibit comparable capacitance behavior and moreover, the inherent capacitance of the Ni NWs is also increased.

Conclusion & Significance: Ni NWs are promising material group for supercapacitor applications similar to Ni foams when they are anodically oxidized by using optimized parameters.

**Recent Publications**

1. Tokmak N and Ürgen M (2017) Production and characterization of electroactive nickel oxides grown on nickel foam by anodic oxidation in KOH melts for supercapacitor application. *MRS Advances* 2(54):3237- 3247.
2. F Bayata, Z Beril Akinci, A Senem Donatan and Mustafa Urgen (2012) A novel free-standing nanowire substrate with surface enhanced Raman scattering (SERS) activity. *Materials Letters* 67(1):387-389.
3. F Bayata and M Ürgen (2015) Role of aluminum doping on phase transformations in nanoporous titania anodic oxides. *Journal of Alloys and Compounds* 646:719–726.
4. F Bayata, B Saruhan-Brings and M Ürgen (2014) Hydrogen gas sensing properties of nano porous al-doped titania. *Sensors Actuators B Chemical* 204:109–118.

5. Z B Akinci and M Urgan (2014) A simple method for the production of aao templates for dc electro deposition of nanostructures. ECS Electro chemistry Letters 3(10):D46–D49.

Biography

Mustafa Ürgen is presently working in the Metallurgical and Materials Engineering Department of Istanbul Technical University and leading the Surface Technologies group. He has more than 130 journal and conference publications. He received best paper award from IMF (International Metal Finishing Society) - Jim Kape Memorial Medal. The innovative coating he has developed in collaboration with Dr. Ali Erdemir (ANL, Chicago-USA) has received the R&D 100 award in 2009. He has given over 25 invited talks in national and international meetings. He took part as Chair and Organization Committee Member in numerous national and international meetings. He has directed several government and industry-sponsored projects and took part in EU funded projects. His research interest areas are: electrolytic, diffusion, PVD and hybrid-PVD coatings, corrosion, nano patterning of surfaces and energy materials. He is one of the authors of 5 issued and 4 pending patents.

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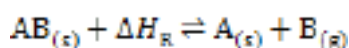
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Materials for thermochemical energy storage: Experimental investigation of cycling stability

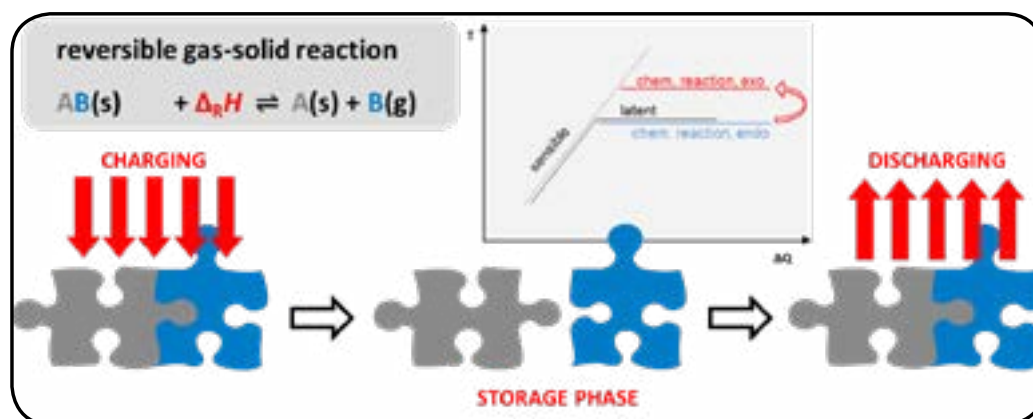
M. Gollsch, J. Stengler, M. Spindler and M. Linder

Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Germany

Thermochemical energy storage (TCS) uses the reaction enthalpy of reversible chemical reactions. This storage technology contains a so far largely untouched potential: in comparison to sensible and latent thermal energy storage, TCS offers potentially higher storage densities, the possibility of long-term storage as well as the option to upgrade the thermal energy. This upgrade can be realised if the reaction system consists of a solid and a gaseous component. For these gas-solid reactions with the generic equation



the equilibrium temperature is dependent on the reaction gas partial pressure: the higher the partial pressure, the higher the reaction temperature. Consequently, the charging of the storage can take place at lower temperatures than the discharging by adjustment of the reaction gas partial pressure. Currently, a number of water vapour-solid reactions are investigated as thermochemical storage materials [1-4]. Apart from a general suitability of a reaction system for thermochemical storage, special attention has to be paid to the cycling stability of the reaction. This is often done using thermogravimetric analysis [5]. However, past scale-ups have shown that behaviour of bulks differs from that of analysis amounts [6]. The bulk's changing properties, however, have proven to be crucial for storage reactor design. The investigation of the cycling stability and reaction behaviour of reacting solid bulks has been our motivation to design and build a cycling test bench. In this experimental setup the gaseous reaction partner is water vapour and can be provided at pressures between 5 kPa and 0.5 MPa. Reactor temperatures can be up to 500 °C. The aim of the presented studies is the automated cycling of about 100 ml solid storage material of reaction systems that have previously shown promise at analysis scale.



Recent Publications

1. Gutierrez, A., Ushak, S., Linder, M. (2018) High Carnallite-Bearing Material for Thermochemical Energy Storage: Thermophysical Characterization. ACS Sustainable Chemistry and Engineering 6(5):6135-6145
2. Afflerbach, S., Kowald, T., Trettin, R. (2017) Phase transformations during de- and rehydration of scholzite $CaZn_2(PO_4)_2 \cdot 2H_2O$. Journal of Solid State Chemistry 254:184-194
3. Stengler, J., Ascher, T., Linder, M. (2017) High temperature thermochemical heat transformation based on $SrBr_2$. 12th IEA Heat Pump Conference, 15th-18th May, 2017, Rotterdam

4. Molenda, M., Stengler, J., Linder, M., Wörner, A. (2013) Reversible hydration behavior of CaCl_2 at high H_2O partial pressures for thermochemical energy storage. *Thermochimica Acta* 260:76-81
5. Richter, M., Habermann, E.-M., Siebecke, E., Linder, M. (2018) A systematic screening of salt hydrates as materials for a thermochemical heat transformer. *Thermochimica Acta* 659:136-150
6. Schaube, F., Kohzer, A., Schütz, J., Wörner, A., Müller-Steinhagen, H. (2013) De- and rehydration of $\text{Ca}(\text{OH})_2$ in a reactor with direct heat transfer for thermos-chemical heat storage. Part A: Experimental results. *Chemical Engineering Research and Design* 91:856-864.

Biography

Marie Gollsch has a degree in environmental engineering and has been at the German Aerospace Center since 2012. She is part of the research area "Thermochemical Systems" at the department of Thermal Process Technology within the Institute of Engineering Thermodynamics. She specialises in the investigation and evaluation of thermophysical properties of thermochemical storage materials with focus on gas-solid reaction systems with water vapour as gaseous component. Additionally, she has expertise in the study of structural changes of the solid components of gas-solid reaction systems which occur due to the cycling of the storage material.

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Notes:

SESSIONS

Nanotechnology and Energy Materials| Solar Energy Materials

Chair: Hyoyoung Lee, Sungkyunkwan University, Republic of Korea

SESSION INTRODUCTION

Title: Flexible reduced graphene oxide based papers: Fabrication and properties

Tseung-Yuen Tseng, National Chiao Tung University, Taiwan

Title: Multi-striped orthogonal photon-photocarrier-propagation solar cells (MOP³SCs) with new asymmetric redirection waveguides

Akira Ishibashi, Hokkaido University, Japan

Title: Active materials for stable perovskite solar cells

Antonio Abate, Helmholtz-Center, Germany

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Flexible reduced graphene oxide based papers: Fabrication and properties

Tseung Yuen Tseng

National Chiao Tung University, Taiwan

A novel way to synthesize flexible and conductive reduced graphene oxide (rGO) based papers is reported. The multi wall carbon nanotubes (MWCNTs) are added into rGO to make rGO/MWCNTs nanocomposite papers. Their electrochemical performance is investigated in various electrolytes, such as KOH, LiOH, and NaOH. The super capacitive behavior of the papers is examined via cyclic voltammetry, galvanostatic charging-discharging and electrochemical impedance spectroscopy. Their physical properties are characterized by X-ray diffractometer, Raman spectrometer, surface area analyzer, thermogravimetric analysis and field emission scanning electron microscope. The rGO/MWCNTs paper synthesized with suitable amount of MWCNTs exhibits excellent performance in KOH with specific capacitance of 200 Fg⁻¹, energy density of 22.5 Whkg⁻¹ and power density of 115 Wkg⁻¹ at current density 0.25 Ag⁻¹. Such high performance of the paper can be used for making future supercapacitors.

Recent Publications

1. Hung C J, Lin P and Tseng T Y (2013) Electrophoretic fabrication and pseudocapacitive properties of graphene/manganese oxide/carbon nanotube nanocomposites. *Journal Power Sources* 243:594-602.
2. Nyholm L, Nyström G, Mihranyan A and Strømme M (2011) Toward flexible polymer and paper-based energy storage devices. *Advanced Materials* 23(33):3751-3769.
3. Gwon H, Kim H S, Lee K U, Seo D H, Park Y C, Lee Y S, Ahn B T and Kang K (2011) Flexible energy storage devices based on graphene paper. *Energy Environment Science* 4:1277-1283.
4. Rath T and Kundu P P (2015) Reduced graphene oxide paper based nanocomposite materials for flexible supercapacitors. *RSC Advance* 5:26666-26674.
5. Kumar N, Kumar A, Huang G M, Wu W W and Tseng T Y (2018) Facile synthesis of mesoporous NiFe₂O₄/CNTs nanocomposite cathode material for high performance asymmetric pseudocapacitors. *Applied Surface Science* 433:1100-1112.

Biography

Tseung Yuen Tseng is a Lifetime Chair Professor in the National Chiao Tung University. He was the Dean of College of Engineering (2005-2007), the Vice Chancellor of the National Taipei University of Technology, Taipei, Taiwan (2007-2009). He has published over 380 research papers in refereed international journals and invented the base metal multilayer ceramic capacitors, which have become large scale commercial product. He has received Distinguished Research Award from the National Science Council (1995-2001), Academic Award of Ministry of Education (2006), National Endowed Chair Professor (2011), and IEEE CPMT Exceptional Technical Achievement Award (2005) and Outstanding Sustained Technical Contribution Award (2012). He was elected a Fellow of the American Ceramic Society in 1998, IEEE Fellow in 2002 and MRS-T Fellow in 2009.

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Multi-striped orthogonal photon-photo carrier-propagation solar cells (MOP³SCs) with new asymmetric redirection waveguides**Akira Ishibashi**

Research Institute for Electronic Science - Hokkaido University, Japan

In orthogonal photon-photo carrier propagation solar cell (MOP³SC), photons propagate in the direction orthogonal to that of the photo carriers. Photons being absorbed in the direction vertical to that of the carrier drift/diffusion, trade-off between photon absorption and carrier collection can be lifted. We can set the stripe-width large enough to absorb all the photons keeping the distance between the p/n electrode distance (= semiconductors layer thickness) short enough to allow most of photo carriers to reach out to the contact metals. Further, by placing those multiple semiconductor stripes, neighboring to each other, with different band-gaps in such an order that the incoming photons first encounter the widest gap semiconductor, then medium-gap ones, and the narrowest at last, we can convert the whole solar spectrum into electricity resulting in high conversion efficiency. The multi-striped solar cell structure is placed at the edge of redirection waveguide in which 3D-propagation photons are redirected to be 2D photons propagating in the waveguide. The waveguide-coupled MOP³SC serves as a concentration photovoltaic system typically operating under a few hundreds to a thousand suns. Using an integrated-paraboloid-sheet as the first layer of the redirection waveguide, we can make the daytime sunlight virtually impinge the rest of the waveguide structure at a right angle. Further, asymmetric waveguide-coupled MOP³SC serves as a highly efficient concentration photovoltaic system thanks to the low temperature rise due to the minimal thermal dissipation and the diffusive light convertibility thanks to the integrated-paraboloid-sheet. The system is also of interest as a high reliability system, because those photons that can damage the bonding of the materials, being converted into electricity already at upstream, never go into the medium or narrow gap semiconductors. Thus, the asymmetric waveguide-coupled MOP³SC would serve as an ultimate high efficiency all-in-one system in the near future.

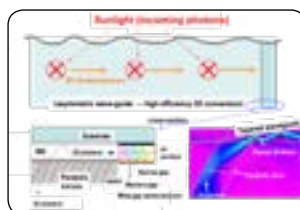


Figure 1: Waveguide-coupled multi-striped orthogonal photon-photo carrier-propagation solar cell (MOP³SC), the cross-section of MOP³SC with the periodic parabolic mirrors (down left), and a simulation result for an example of asymmetric waveguide [tapered WG] (down right). The total width of the multi-striped semiconductor is tens to hundreds of microns.

Recent Publications

1. Ishibashi A, White S, Kawaguchi N, Kondo K and Kasai T (2016) Edge-illumination scheme for multi-striped orthogonal photon-photo carrier - propagation solar cells, *Int. J. Eng. Tech. Res.* 6(1):115-117.
2. Ishibashi A, Kobayashi H, Taniguchi T, Kondo K and Kasai T (2016) Optical simulation for multi-striped orthogonal photon - photo carrier-propagation solar cell (MOP³SC) with redirection waveguide. *3D Research* 7:33.
3. Ishibashi A (2016) Orthogonal photon-photo carrier - propagation solar cells, (in Japanese) *Energy Devices* 3(4): pp. 77-83.

Biography

Akira Ishibashi received the BSc, MSc and PhD degrees in Physics in 1981, 1983, and 1990, respectively, all from the University of Tokyo, Japan. During 1982–1983, he was a Research Assistant at LBNL, Berkeley, USA. In 1983, he joined the Research Center of Sony Corporation, Yokohama. He was a Visiting Faculty at Loomis Laboratory, Department of Physics, University of Illinois at Urbana-Champaign, 1990-1991. In Sony he achieved world-first RT CW operation of blue/green laser diodes using ZnMgSSe, in 1993. He was a Visiting Professor at Center for Interdisciplinary Research, Tohoku University, Japan in 1998. Since 2003 he has been a full Professor in leading Nanostructure Physics Lab in RIES, Hokkaido University, Japan. In 2006, he started Hokkaido University Venture Company, C'sTEC Corp., based on Clean Unit System Platform (CUSP). His main target is to realize high-efficiency solar cells exploiting CUSP that helps people live in a high standard.

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Scientific Tracks & Abstracts Day 2

Advanced Energy Materials 2018

SESSIONS

Polymer Materials| Electrical, Optical and Magnetic Materials| Mining, Metallurgy and Materials Science

Chair: Antonio Di Bartolomeo, University of Salerno, Italy

SESSION INTRODUCTION

- Title:** Graphene-Silicon Schottky heterojunctions for optoelectronic applications
Antonio Di Bartolomeo, University of Salerno, Italy
- Title:** Polyacetylene: Myth, reality and a way forward
Bruce S. Hudson, Syracuse University, USA
- Title:** A sustainable technology for extraction of cobalt and nickel from laterite ores
Guangqing Zhang, University of Wollongong, Australia
- Title:** The phenomenological energy model of orthotropic nonlinear elastic material on the example of rolled sheet of cylindrical tank
Maciej Obst, Poznan University of Technology, Poland
- Title:** The modeling of selected mechanical properties of plastic materials under influence of complex external load state
Dariusz Kurpisz, Poznan University of Technology, Poland

Graphene-silicon Schottky heterojunctions for optoelectronic applicationsAntonio Di Bartolomeo¹, Giuseppe Luongo¹, Laura Iemmo¹, Francesca Urban¹ and Filippo Giubileo²¹Università di Salerno, Italy²CNR-SPIN, Italy

The graphene/silicon (Gr/Si) junction has been the subject of an intense research activity both for the easy fabrication and for the variety of phenomena that it allows studying. It offers the opportunity to investigate new fundamental physics at the interface between a 2D semimetal and a 3D semiconductor, and holds promises for a new generation of graphene-based devices such as photodetectors, solar cells and chemical-biological sensors. A Gr/Si junction with defect-free interface exhibits rectifying current-voltage (I-V) characteristics, which are the result of the formation of a Schottky barrier, as in traditional metal-semiconductor (M/S) Schottky diodes. The vanishing density of states at the graphene Dirac point enables Fermi level tuning and hence Schottky barrier height modulation by a single anode-cathode bias. When the Gr/Si junction is used as a photodiode, graphene acts not only as anti-reflecting and transparent conductive layer for charge transport to the external circuit, but it functions also as active material for light absorption and electron-hole generation and separation. Although most of the incident light is converted to photocharge into Si, the absorbance in graphene enables detection of photons with Si sub-bandgap energy through internal photoemission over the Schottky barrier. Photo charges injected over the Schottky barrier, under high reverse bias, can be accelerated by the electric field in the depletion region of the diode and cause avalanche multiplication by scattering with the Si lattice, thus enabling internal gain. The Gr/Si junction forms the ultimate ultra-shallow junction, which is ideal to detect light absorbed very close to the Si surface, such as near- and mid-ultraviolet. In this talk, we present the electrical characterization and the photoresponse of two types of Gr/Si devices, shown in figures 1 (b) and (c). Although due to different mechanisms, on both devices we demonstrate photo-responsivity exceeding 2.5 A/W that is competitive with present solid-state devices. We attribute it to the contribution of charges photogenerated in the surrounding region of the flat junction or to the internal gain by impact ionization caused by the enhanced field on the nano tips.

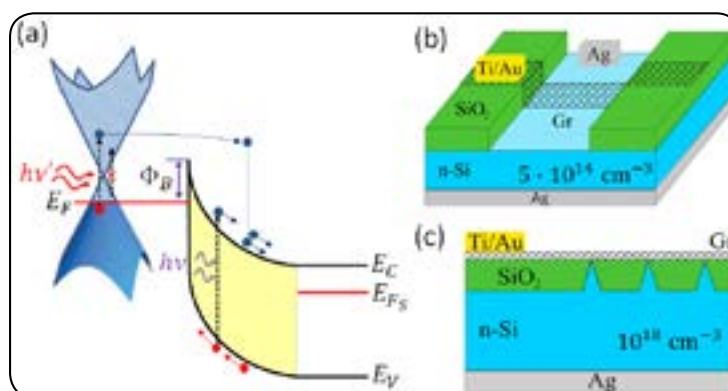


Figure 1: (a) Photodetection in a Gr/Si junction. Photons with energy lower than the Si bandgap, $E_0 = E_c - E_v$, but higher than the Schottky barrier Φ_b ($\Phi_b < h\nu < E_0$) can be absorbed in graphene. Emitted over the Schottky barrier, such electrons can originate avalanche multiplication through impact ionization. (b) Graphene on flat Si substrate ("flat Gr/Si" junction) and (c) graphene on patterned Si (Gr/Si-tips junction)

Recent Publications:

1. Di Bartolomeo A (2016) Graphene Schottky diodes: An experimental review of the rectifying graphene/semiconductor heterojunction. Physics Reports 606:1-58.

2. Di Bartolomeo A, Luongo G, Giubileo F, Funicello N, Niu G, Schroeder T, Lisker M and Lupina G (2017) Hybrid graphene/silicon Schottky photodiode with intrinsic gating effect. *2D Materials* 4:025075
3. Luongo G, Giubileo F, Genovese L, Iemmo L, Martucciello N and Di Bartolomeo A (2017) I-V and C-V characterization of a high-responsivity graphene/silicon photodiode with embedded MOS capacitor. *Nanomaterials* 7(7):158
4. Di Bartolomeo A, Giubileo F, Luongo G, Iemmo L, Martucciello N, Niu G, Fräschke M, Skibitzki M, Schroeder T and Lupina G (2017) Tunable Schottky barrier and high responsivity in graphene/Si-nanotip optoelectronic device. *2D Materials* 4(1):015024.
5. Giubileo F and Di Bartolomeo A (2017) The role of contact resistance in graphene field-effect devices. *Progress in Surface Science* 92(3):143-175.

Biography

Antonio Di Bartolomeo received MS and PhD degree in Physics from Salerno University, Italy. He worked as System Engineer for Creative Electronic Systems (CH) and as Device Engineer for ST Microelectronics (AZ) and Intel Corporation (IE). He started his career in experimental high-energy physics in the CHORUS and ALICE experiments at the CERN (Geneva, CH). Currently, he works as Associate Professor of Experimental Condensed Matter Physics at the Salerno University, Italy. He has been Visiting Scientist at IHP Microelectronics, Frankfurt Oder, Germany, and at the Georgetown University, Washington, DC. He has co-authored two textbooks on general Physics and more than 80 peer-reviewed research articles and is in the Editorial Board of Nanotechnology (IOP) and Nanomaterials (MDPI). His present research interests include: Optical and electrical properties of carbon nanotubes, graphene, 2D materials and composite materials; graphene/semiconductor heterojunctions and their application as photodetectors, solar cells and chemical sensors; Van der Waals heterojunctions of 2D layered materials; field-effect transistors; tunneling transistors; non-volatile memories; CMOS technologies; solid-state radiation detectors; field emission.

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Notes:

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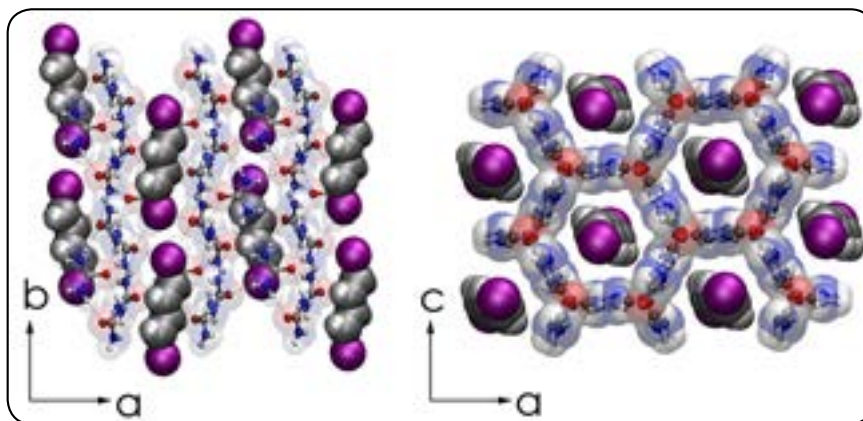
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Polyacetylene: Myth, reality and a way forward

Bruce S Hudson

Syracuse University, USA

Polyacetylene, the simplest and oldest conducting polymer, has never been made in a form that permits rigorous determination of its structure. Trans polyacetylene will have two equivalent potential energy minima. It has been assumed that this results in bond length alternation. It is, however, very likely that the zero-point energy is above the Peierls barrier. Experimental studies that purport to show bond alternation have been reviewed and shown to be compromised by experimental inconsistencies or by the presence of finite chain polyenes. This situation has been reviewed in an open paper. A method for preparation of high molecular weight polyacetylene with fully extended chains that are prevented from reacting with neighboring chains by photochemical polymerization of a reactive guest molecule in urea inclusion complexes (UICs) is then discussed. The structural chemistry of these UIC materials will be reviewed. Our current projects involve guest species diiodo butadiene or diiodo hexatriene. The loss of iodine atoms during the elimination polymerization is monitored by weight loss. The polyacetylene chains form in UIC channels as fully extended chains that are parallel with a separation of 0.82 nm in a hexagonal lattice. The diene and triene guest species differ in crystal morphology with the triene presenting with hexagonal needles. Raman spectroscopy used to monitor the formation of polyene chains suffers losses of intensity when the chains are very long. The final material is characterized by vibrational inelastic neutron scattering using VISION at the Oak Ridge National Laboratory. Our ultimate objective is to measure electrical conduction of polyacetylene in urea inclusion compounds along the *c*-axis of the hexagonal channel. The strong bonding of carbon atoms suggests that this material may be a superconductor at room temperature due to the lack of thermally populated phonons. Methods for the formation of closed loop structures are being considered.



Recent Publications:

1. Hudson B S and Allis D G (2013) Bond alternation in infinite periodic polyacetylene: dynamical treatment of the anharmonic potential. *Journal of Molecular Structure* 1032:78-82.
2. Dinca S A, Allis D G, Lashua A F, Sponsler M B and Hudson B S (2015) Insulated polyacetylene chains in an inclusion complex by photo polymerization. In *Crystal Engineering - Design, New Materials and Application* 1799:7-12.
3. Lashua A F, Smith T M, Hu H, Wei L, Allis D G, Sponsler M B and Hudson B S (2013) Commensurate urea inclusion crystals with the guest (e,e) 1,4-diiodo-1,3-butadiene. *Crystal Growth & Design* 13:3852-3855.

4. Marti Rujas J, Desmedt A, Harris K D M and Guillaume F (2009) Bidirectional transport of guest molecules through the nanoporous tunnel structure of a solid inclusion compound. *Journal of Physical Chemistry A* 113:736–743.
5. Hudson B S (2001) Oriented n-alkanes in urea-d₄ inclusion complexes for inelastic neutron scattering vibrational studies. *Molecular Crystals and Liquid Crystals* 356:423-432.

Biography

Bruce S Hudson received his Bachelor's and Master's degrees in Biophysical Chemistry from the California Institute of Technology in Pasadena, California and his PhD degree in Physical Chemistry from Harvard University where he worked for Bryan E Kohler on the peculiar electronic spectroscopy of linear conjugated polyenes. As part of his PhD thesis he proposed that the lowest excited electronic state of linear polyenes has the same symmetry as the ground electronic state involving doubly excited configurations. It is the merging of this excited state with the ground state for very long linear polyenes that gives rise to the double minimum potential of polyacetylene. He is a fellow of the American Physical Society.

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A sustainable technology for extraction of cobalt and nickel from laterite ores

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Cobalt and nickel are two of the key base metals for the production of high energy density batteries. Their availability and costs are key factors that will determine the success in popularizing electric vehicles in the future. This paper presents a potential technology for sustainable extraction of cobalt and nickel from laterite ores. The major phases in a garnierite laterite ore include chlorite, talc, hematite, and quartz. In the technology, cobalt and nickel oxides are selectively reduced in a controlled atmosphere to their metal states while the reduction of iron oxides is minimized. At 740°C in 60 vol.% CO-40 vol.% CO₂, 91% Ni and 94% Co in the particles <53 μm and 85% Ni, 99% Co in the particles 53-200 μm but less than 20% Fe are reduced to metals. The reduced metals are then carbonylated by carbon monoxide in a pressurized reactor at ~100°C. Using sulfur as a catalyst and under CO pressure of 15 atm., 97% of nickel from reduction of NiO is carbonylated. The conditions for the carbonylation of nickel from reduced laterite ore needs to be optimized. The reduced nickel and iron are separated from the ore due to formation of volatile carbonyls, and are recovered from the carbon monoxide stream. Cobalt carbonyl left with the reduced ore is further separated by vaporization or dissolution and recovered as metal product. The proposed technology has the advantages of low energy costs and low production costs, and so will be suitable for the extraction of cobalt and nickel from the low-grade laterite ores which will expand the cobalt and nickel resources, and so contributes to the sustainable development of the related metals and their applications.

Recent Publications:

1. Olivetti E A, Ceder G, Gaustad G G and Fu X (2017) Lithium-ion battery supply chain considerations: analysis of potential bottlenecks in critical metals. *Joule* 1(2):229-243
2. Yang J, Zhang G, Ostrovski O and Jahanshahi S (2013) Changes in an Australian laterite ore in the process of heat treatment. *Minerals Engineering* 54:110-115.
3. Yang J, Zhang G, Jahanshahi S and Ostrovski O (2015) Reduction of a garnieritic laterite ore by CO-CO₂ gas mixtures. *INFACON XIV* 518-527.

Biography

Guangqing Zhang has expertise in the development of sustainable technologies for metals production. He has applied the kinetics and thermodynamics and engineering knowledge in the development of alternative technologies and improvement of current technologies for metals production. His research fields include process metallurgy, energy conversion, and recycling of waste materials.

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The phenomenological energy model of orthotropic nonlinear elastic material on the example of rolled sheet of cylindrical tank

Maciej Obst and Dariusz Kurpisz
Poznan University of Technology, Poland

The orthotropic materials are one of the most important construction elements. In many cases the orthotropic is the relic of technological process like plate rolling. Because the mechanical properties of such type of material depend on the chosen sheet rolling direction, the ability to predict the strength situation is very important, when the material will be destroyed. Very useful can be the strain energy based methods which were used among others in papers and sheet rolling direction of sheet metal and mechanical properties changes can be important when loaded part of device is under dynamic impacts. Fatigue processes initiation depends also on local material properties differences and micro notches. The authors of the presentation applied the strain energy density function for the analytical description of the behaviour of orthotropic material forced in plane state of stress. The described investigation results are presented on a practical example of the back surface of the thin-walled cylindrical tank under the influence of internal pressure. The material stability assumptions formulated on the basis of the strain energy density function, will be very useful and important in the prediction of failure of material due to a plastic flow and particularity in the assessment of strength of the responsible cylindrical shell. As mentioned, dynamic impacts and fatigue phenomena depend on local material properties and notches shapes. Strain energy based method proposed by authors can be developed and helpful for researchers and engineers interested in the design of the responsible constructions. The proposed energy method is universal and can be modified for the investigated model of construction and applied materials also unconventional materials such as composites or polymers.

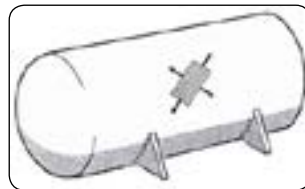


Figure 1: Orthotropic tank

Recent Publications:

1. Wegner T (2000) Surface of limit state in nonlinear material and its relation with plasticity condition. *The Archive of Mechanical Engineering* 47(3):205-223.
2. Wegner T and Kurpisz D (2013) Phenomenological modelling of mechanical properties of metal foam. *Journal of Theoretical and Applied Mechanics* 51(1):203-214.
3. Obst M, Kurpisz D and Paczos P (2016) The experimental and analytical investigations of torsion phenomenon of thin-walled cold formed channel beams subjected to four-point bending. *Thin-Walled Structures* 106:179-186.
4. Obst M, Kurpisz D and Mencil K (2015) Energy based mechanical characteristics of polymers POM-C, PET, PA6, PVC, PVDF. *Machine Dynamics Research* 39(4):93-106.
5. Obst M, Rodak M and Paczos P (2016) Limit load of cold formed thin-walled nonstandard channel beams. *Journal of Theoretical and Applied Mechanics* 54(4):1369-1377.

Biography

Maciej Obst is a Scientific Worker at the Poznan University of Technology. His scientific interests include experimental and analytical research of mechanical properties of materials, dynamics, constructions and complex structures where strength of materials, mechanics and energy dependences are used for analysis and research. His scientific activity also includes automotive technology, transportation problems, applied mechanical engineering directed to material properties, stress and strain dependences, energy distribution. Research experience and academic activity are energy based method material properties modeling, material properties experimental research, construction experimental research such as car seat belts, lashing straps, suspension air springs, brakes and friction research, scientific experimental stands design and other interesting devices.

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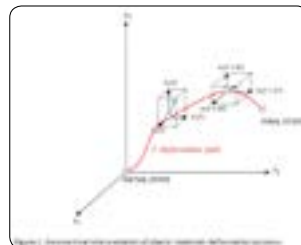
The modeling of selected mechanical properties of plastic materials under influence of complex external load state

Dariusz Kurpisz and Maciej Obst
Poznan University of Technology, Poland

One of the most important and widely used materials is plastic materials. Hence, the knowledge on the behaviour and especially mechanical properties of this type of materials plays an important role in their strength assessment. Very important is here the practical possibility of the prediction of material behaviour under the influence of complex load state; where useful and very important are the strain energy based methods of mechanical properties modelling of material. Such type of approach to the modelling was used by Kurpisz and Wegner among others in [4] and [5]. In the current paper basing on phenomenological approach and interpretation of mechanical experimental characteristics, the strain energy model of plastic material under complex load state in range of elastic deformations, will be introduced. The strain energy density function which is a density of the work of stress components $\sigma_i(t)$ for $i=1,2,3$ along deformation path $C:\varepsilon_i(t)$ for $i=1,2,3$ defined in the form:

$$W(\varepsilon_1, \varepsilon_2, \varepsilon_3) = \int \sum_{i=1}^3 \sigma_i d\varepsilon_i = \int_0^1 \sum_{i=1}^3 \sigma_i(t) \varepsilon'_i(t) dt.$$

will be applied for determination of material stability assumption due to the possibility of the appearing of plastic flow. All theoretical investigations will be illustrated on the example of two types of plastics materials in three-axial state of stress.



Recent Publications:

1. Li Q M (2001) Strain energy density failure criterion. *International Journal of Solids and Structures* 38(38-39):6997-7013.
2. Valavala P K, Odegerd G M (2007) Multiscale constitutive modeling of polymer materials, *ASME 2007 International Mechanical Engineering Congress and Exposition*, 179-183.
3. W Y J, Li J and Faria R (2006) An energy release rate-based plastic-damage model for concrete. *International Journal of Solids and Structures* 43:583-612.
4. Wegner T and Kurpisz D (2013) Phenomenological modeling of mechanical properties of metal foam. *Journal of Theoretical and Applied Mechanics* 51(1):203-214.
5. Wegner T and Kurpisz D (2017) An energy-based method in phenomenological description of mechanical properties of nonlinear materials under plane stress. *Journal of Theoretical and Applied Mechanics* 55(1):129-139.

Biography

Dariusz Kurpisz is a scientific worker at the Poznan University of Technology. His scientific interest includes mathematical modeling of physical process both for materials as well for more complicated structures. One of the most important tools in his work are phenomenological approach and energy method of modeling based on experimental approach and the strain energy density function.

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SESSIONS

Advanced Nanomaterials |Advanced Graphene Materials| Hydrogen Energy

Chair: Jerzy. A. Szpunar, University of Saskatchewan, Canada

SESSION INTRODUCTION

Title: Recent progressive of two-dimensional materials for terahertz detection

Lin Wang, Shanghai Institute of Technical Physics, China

Title: Towards sensitive terahertz detection via thermoelectric manipulation in graphene transistors

Gang Chen, Shanghai Institute of Technical Physics, China

YRF

YRF: Superior hydrogenation/dehydrogenation kinetics of MgH_2 nanopowders upon mechanical doping with amorphous Zr_2Ni

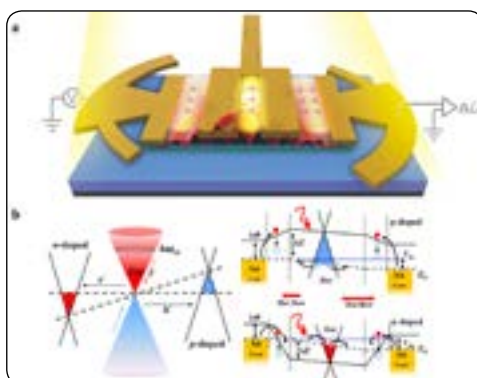
Fahad Al-Ajmi, Kuwait Institute for Scientific Research, Kuwait

YRF: Window ventilation system with Artificial neural network for reducing fine dust indoors

Young Kwon Yang, Chung-Ang University, South Korea

Recent progressive of two-dimensional materials for terahertz detectionLin Wang^{1,2}, Xiaoshuang Chen^{1,2} and Wei Lu²¹Shanghai Institute of Technical Physics - Chinese Academy of Sciences, China²University of Science and Technology of China, China

Recent years, layered van der Waals (vdW) crystals consist of individual atomic planes weakly coupled by vdW interaction have attracted great interests due to their intriguing physical properties, such as superconductivity, high carrier mobility, topologically protected surface states and among many others. An ambitious practical goal is to exploit planes of vdW crystals as building blocks of more complex optoelectronic application, especially in the terahertz band. The pursuit of two-dimensional materials for terahertz detection is promoted by the unique properties beyond traditional system, such as good CMOS-compatibility, easy for fabrication and fast response. Especially, graphene can support terahertz plasmon which can lead to enhanced THz absorption. Graphene-based terahertz detectors rely on the photo thermoelectric and self-mixing effects both of these effects depends on the near-field or the decay of plasmons. Also, other two-dimensional materials such as black phosphorus, topological insulator exhibit exotic THz optoelectronic properties, such as anisotropic band structure in black phosphorus (BP), interplay between surface states and bulk states such as in Bi_2Se_3 exhibiting the unique THz spectral profile. Initial characterization has demonstrated the excellent interaction between THz photons and two dimensional materials. However, convert absorbed photons into electricity with high efficiency is still a big challenge. In typically, self-mixing process for direct detection require materials with both high mobility and moderated bandgap, and is usually wipe out/disrupted by the coexisting mechanism such as thermoelectric process. In this work, we present a new route toward manipulation of hot electrons within high mobility materials such as BP and graphene. Due their moderated bandgap, the hot electrons in atomic plane can be extensively excited and randomized. The unilateral flow of excess hot electrons can be facilitated by exploring both the electromagnetic engineering and electrostatic tuning. Intriguingly, the hot electrons effect changes the resistance via nonequilibrium carrier diffusion, leading to the high photoelectric gain under electrical bias. The present results and the novel hot electron mechanism allow for realistic exploitation of two-dimensional materials for large area, fast imaging.

**Recent Publications:**

1. L Vicarelli, M S Vitiello, D Coquillat, A Lombardo, A C Ferrari, W Knap, M Polini, V Pellegrini and A Tredicucci (2012) Graphene field-effect transistors as room-temperature terahertz detectors. *Nature Materials* 11:865-871.
2. Lin Wang, Changlong Liu, Xiaoshuang Chen, Jing Zhou, Weida Hu, Xiaofang Wang, Jinhua Li, Weiwei Tang, Anqi Yu and Shao Wei Wang (2017) Toward sensitive room-temperature broadband detection from infrared to terahertz with antenna-integrated black phosphorus photoconductor. *Advanced Functional Materials* 27(7):1604414.
3. Changlong Liu, Lin Wang, Xiaoshuang Chen, Jing Zhou, Weida Hu, Xinran Wang, Jinhua Li, Zhiming Huang, Wei Zhou, Weiwei Tang, Gangyi Xu, Shao-Wei Wang and Wei Lu (2018) Room-temperature photoconduction assisted by hot-carriers in graphene for sub-terahertz detection. *Carbon* 130:233-240.

4. Weiwei Tang, Antonio Politano, Cheng Guo, Wanlong Guo, Changlong Liu, Lin Wang, Xiaoshuang Chen and Wei Lu (2018) Ultra-sensitive room-temperature terahertz direct detection based on bismuth selenide topological insulator. *Advanced Functional Materials* DOI:10.1002/adfm.201801786.
5. Changlong Liu, Lin Wang, Xiaoshuang Chen, Jing Zhou, Weiwei Tang, Wanlong Guo, Jin Wang and Wei Lu (2018) Top-gated black phosphorus phototransistor for sensitive broadband detection. *Nanoscale* 10(13):5852-5858.

Biography

Lin Wang is currently an Associate Professor in Shanghai Institute of Technical Physics, Chinese Academy of Science. He has been awarded many prizes including special prize of president scholarship for distinguished postgraduate student. He received the outstanding achievement award in Shanghai. He has authored or coauthored more than 40 technical journal papers and delivered more than 10 invited conference presentations, serving as a journal peer-reviewer in *Advanced Functional Materials*, *ACS Nano*, *APL*, etc. His current research interests include plasma wave detection of terahertz/infrared radiation using graphene and III-V, plasmonic nanomaterials and metamaterials devices, graphene-like two-dimensional optoelectronics.

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Towards sensitive terahertz detection via thermoelectric manipulation in graphene transistors

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Graphene has been highly sought-after as a potential candidate for hot electron terahertz (THz) detection benefiting from its strong photon absorption, fast carrier relaxation and weak electron-phonon coupling. Nevertheless so far graphene based thermoelectric THz photo detection is still hindered by the low responsivity owing to the relatively low photo-electric efficiency. In this work, we provide a straightforward strategy for the enhanced THz detection based on antenna-coupled CVD graphene transistors with the introduction of symmetric paired fingers. This design enables switchable photo detection modes by controlling of the interaction between the THz field and free hot carriers in graphene channel through different contacting configurations. Hence a novel bias field effect can be activated which leads to a drastic enhancement in THz detection ability with responsivity up to 280 V/W and Johnson-noise limited minimum noise-equivalent power (NEP) of 100 p W/Hz^{0.5} at room temperature. The mechanism of the enhancement of the photoelectric gain is attributed to the thermo photovoltaic instead of the plasma self-mixing effects; our results offer a promising alternative route to scalable, wafer-level production of high performance graphene detectors.



Recent Publications:

1. Liu D, et al. (2018) Efficient Raman enhancement on high-quality ultra-clean graphene quantum dots produced by a quasi-equilibrium plasma-enhanced chemical vapor deposition. *Nature Communications* 9:193.
2. Liu C, et al. (2018) Towards sensitive terahertz detection via thermoelectric manipulation in graphene transistors. *NPG Asia Materials* 10:318-327.
3. Du L, et al. (2018) Thickness-controlled direct growth of nanographene and nanographite film on non-catalytic substrates. *Nanotechnology* 29(21):215711.
4. Sun F, et al. (2018) Optical waveguide of buckled CdS nanowires modulated by strain engineering. *ACS Photonics* 5:746-751.
5. Du L, et al. (2017) Formation of Self-connected Si^{0.8}Ge^{0.2} lateral nanowires and pyramids on Rib-patterned Si (1 1 10) substrate. *Nanoscale Research Letters* 12:70.

Biography

Gang Chen has his expertise in growth of semiconductor materials and the fabrication of opto electronic devices. He received his PhD on Condensed Matter Physics from Fudan University, Shanghai, China in 2002. Then he had been working at the Institute of Solid State Physics in Johannes Kepler University, Linz, Austria for ten years on the MBE growth of SiGe based nanostructures and their application in the optoelectronics. Now he is a Professor in Chinese Academy of Sciences, Shanghai Institute of Technical Physics. He has published more than 60 research papers in peer-reviewed journals. His main research interest is on the field of the fabrication low dimensional carbon allotrope and their application on ultra-broad photo detection.

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Superior hydrogenation/dehydrogenation kinetics of MgH₂ nanopowders upon mechanical doping with amorphous Zr₂Ni

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Hydrogen is an energy carrier, which holds tremendous promise as a new clean energy option. Hydrogen storage, which is considered to be the most important factor cutting across both hydrogen production and hydrogen transportations, has been the subject of intensive research for many years. Mg and Mg-based materials have opened promising concept for storing hydrogen in a solid-state matter. The natural abundance, cheap price, operational cost effectiveness, light weight, and high hydrogen storage capacity (7.60 wt.%, 0.11 kg H₂L⁻¹) are some advantages of Mg and Mg-based alloys making them desirable storage materials for research and development. Whereas all catalytic materials used to improve the behaviors of hydrogenation/dehydrogenation kinetics for MgH₂ have long-range order structure, the present work proposes two different types of structure; i.e. short range- and medium range- order. For the purpose of the present study, MgH₂ powders were prepared by reactive ball milling of Mg powders under 50 bar of H₂, using room-temperature high-energy ball mill [5]. Ultrafine powders of amorphous- and big cube-Zr₂Ni phases were prepared by ball milling small bulk pieces of tetragonal-Zr₂Ni alloy prepared by arc melting technique. Small volume fraction (10 wt. %) of amorphous and big- cube powders obtained after ball milling for 100 and 150 h, respectively were individually mixed with as-synthesized MgH₂ powders and then ball milled for 50 h. The results have shown that nanocomposite MgH₂/10 wt.% metallic glassy Zr₂Ni powders had high density of hydrogen (~6 wt.%) and possessed fast kinetics of hydrogen uptake/release at 250°C within 1.15 and 2.5 min, respectively. Whereas, MgH₂/10 wt.% of big cube Zr₂Ni nanocomposite showed moderate improvement on hydrogenation (1.8 min)/dehydrogenation (7 min) kinetics due to the heterogeneous distribution of their particles onto the MgH₂ powders.

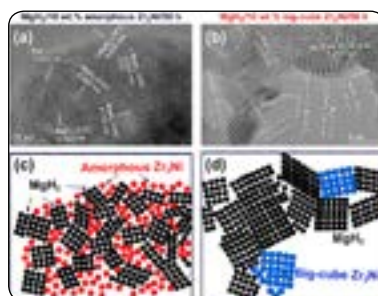


Fig. HRTEM images of nanocrystalline MgH₂ powders doped with 10 wt.% of (a) amorphous Zr₂Ni, and (b) big-cube Zr₂Ni nanopowders. The corresponding illustration sketches for the HRTEM images shown in (a) and (b) are displayed in (c) and (d), respectively.

Recent Publications:

1. El-Eskandarany, M. Sherif (2017) Synthetic nanocomposite MgH₂/5 wt. % TiMn₂ powders for solid hydrogen storage tank integrated with PEM fuel cell Nature, Sci. Rep. 7: 13296; doi: 10.1038/s41598-017-13483-0. www.nature.com/scientificreports.
2. El-Eskandarany, M. Sherif et al. (2017) Structure, morphology and hydrogen storage kinetics of nanocomposite MgH₂/10 wt% ZrNi₅ powders, Materials Today Energy, 3: 60-71.
3. El-Eskandarany, M. Sherif et al. (2016) In-situ catalyzation approach for enhancing the hydrogenation / dehydrogenation kinetics of MgH₂ powders with Ni particles. Sci. Rep. 6, 37335; DOI: 10.1038/srep37335 www.nature.com/scientificreports.
4. El-Eskandarany, M. Sherif (2016) Metallic glassy Zr₇₀Ni₂₀Pd₁₀ powders for improving the hydrogenation/dehydrogenation behavior of MgH₂. Nature, Sci. Rep. 6, 26936; doi: 10.1038/srep26936. www.nature.com/scientificreports.

5. El-Eskandarany M.Sherif, Shaban E., Alsairafi A. (2016) Synergistic dosing effect of TiC/FeCr nanocatalysts on the hydrogenation/dehydrogenation kinetics of nanocrystalline MgH₂ powders. Energy 104: 158-170.

Biography

Fahad Al-Ajmi works at Kuwait Institute for Scientific Research KISR in the Nanotechnology and Advanced Materials department. He obtained his master degree in advanced chemical engineering from the University of Manchester, and the bachelor degree in chemical engineering from Swansea University UK.

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Notes:

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Window ventilation system with artificial neural network for reducing fine dust indoors

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This study proposes a window ventilation system according to the of indoor and outdoor air quality. system artificial intelligence (AI) ventilation monitor indoor and outdoor air quality in real time based on the Internet of Things (IoT). maximizes ventilation efficiency Bernoulli's principle. The study results of this study are as follows: designed to create comfortable indoor environments using weather and air quality information. functions applied. First, AI technology used to predict the ventilation operation according to indoor . based IoT used to monitor indoor and outdoor in real time. Bernoulli's principle used to maximize the ventilation efficiency. The AI-based window ventilation system is expected to respond to various environmental changes to improve indoor air quality. can minimize building energy consumption automatically ventilation.



Fig. 1.1 Comparison of operation between existing ventilation and window ventilaton with artificial intelligence



Fig. 1.2 Artificial intelligent Window ventilation system.

Recent Publications:

1. 2015, Effect of the solar radiative properties of existing building roof materials on the energy use in humid continental climates, [Energy & Buildings]
2. 2016, Development of PCM cool roof system to control urban heat island considering temperate climatic conditions [Energy & Buildings]
3. 2016, Development of a small wind power system with an integrated exhaust air duct in high-rise residential buildings, [Energy & Buildings]
4. 2017, Proposal of a PCM underfloor heating system using a web construction method, [International journal of polymer science]
5. 2017, Effect of PCM cool roof system on the reduction in urban heat island phenomenon, [Building & Enveironment].

Biography

Young Kwon Yang is currently a PhD candidate with the Centre for Sustainable Architecture and Building Systems Research at Chung-Ang University. Yang obtained patents for auto-ventilation systems, latent heat of phase change materials and solar heat exchange system, and phase change materials as roof finishing materials while completing a doctoral course in 2016-2017.

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