2017 ESS Safety Forum to be held February 22–24 in the United States

https://share.sandia.gov/ess/ess-safety-forum-2017

Meeting the Challenge: 2017 Energy Storage System Safety Forum (2017 ESS Safety Forum) will be held February 22–24, 2017, in New Mexico, USA.

The main objective is to provide a platform to discuss the current state of ESS safety and mitigation strategies for improving cell to system safety and reliability. This open forum will allow researchers an opportunity to present their work in ESS, including research and development, code standards and regulations (CSRs), as well as gaps in CSRs that affect deployment of energy storage. This will encompass, but is not limited to, developing inherently safe battery chemistries, energy-storage software, power electronics and cyber security to improve safety and monitoring, designing safe systems, codes and standards, signage, and commissioning.

More information can be accessed from the forum website at https://share.sandia.gov/ess/ess-safety-forum-2017 or by email at ESSforum@sandia.gov.

OP2017 to be held June 19–23 in Canada

http://op2017.org

The 12th International Conference on Optical Probes of Organic and Hybrid Semiconductors (OP2017) will be held June 19–23, 2017, in Québec City, Canada. The co-chairs are Carlos Silva of Université de Montréal, Canada; and Stéphane Kéna-Cohen of École Polytechnique de Montréal, Canada.

The scope of the conference is a variety of excited state phenomena in technologically important materials and biosystems, including size-dependent and time-dependent electronic interactions, excited state dynamics, strong light–matter interactions, quantum confinement, photocarrier transport, and novel spectroscopic techniques. The objective is to place emphasis on the generality of the phenomena rather than specifics of the systems and optical measurements.

Topics include

- Organic and polymeric materials (photophysics, chemistry, and dynamics)
- Energy transport and exciton annihilation processes
- Organic/polymeric electronic devices (OLEDS, OPV)
- Photophysics and applications of hybrid organometal perovskite materials
- Thermally activated delayed fluorescence in OLEDs
- Organometallic complexes (photophysics and applications)
- Semiconductor nanocrystals and metal nanoparticles (hybrid devices and novel physical phenomena)
- Organic and inorganic nanostructured photovoltaic phenomena (physics, chemistry, and devices)
- Optical properties of carbon allotropes
- Photophysics of 2D atomic-layered materials
- Molecular and supramolecular ordered assembly at nanoscales
- Novel optical probes for condensed-matter materials research
- Singlet fission
- Spin dynamics in organic systems
- Photophysics of bioorganic materials and luminescent optical probes

Confirmed plenary speakers are Vahid Sadoghdar of the Max Planck Institute for the Science of Light, and Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Chihaya Adachi of Kyushu University, Japan; and Greg Scholes of Princeton University, USA.

The abstract submission deadline is February 29. The early bird and presenting author registration deadline is April 18. More information can be accessed from the conference website at http://op2017.org or by email at OP2017@conferium.com.

YUCOMAT 2017 to be held September 4–8 in Montenegro

www.mrs-serbia.org.rs/index.php/yucomat-2017m

YUCOMAT 2017 will be held September 4–8, 2017, in Herceg Novi, Montenegro. It is organized by the Materials Research Society of Serbia.

Five symposia will comprise invited plenary lectures, oral presentations, and poster presentations: Symposium A—Advanced Methods in Synthesis and Processing of Materials; Symposium B—Advanced Materials for High-Technology Application; Symposium C—Nanostructured Materials; Symposium D—Eco-Materials and Eco-Technologies; and Symposium E—Biomaterials. The conference will also feature a tutorial for young researchers and an exhibition of synthesis and characterization equipment.

Awards will be presented to the authors (preferably members younger than 35) of the best oral and poster presentation at the conference, and also to the authors of highly rated PhD theses defended between two conferences.

The deadline for abstract submission is May 1. Preregistration ends June 15, and regular registration ends July 31. More information can be accessed from the conference website at www.mrs-serbia.org.rs/index.php/yucomat-2017m or by email at yucomat@mrs-serbia.org.rs. □

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SPECIAL ISSUE PROSPECTIVE ARTICLES: FUNCTIONAL OXIDES

Nanostructured cerium oxide: preparation, characterization, and application in energy and environmental catalysis

Wen-Xiang Tang and **Pu-Xian**, University of Connecticut, USA

Nanostructured cerium oxide (CeO_2) with outstanding physical and chemical properties has attracted extensive interests over the past few decades in environment and energy-related applications. With controllable synthesis of nanostructured CeO_2, much more features were technologically brought out from defect chemistry to structure-derived effects. This review highlights recent progress on the synthesis and characterization of nanostructured ceria-based materials as well as the traditional and new applications. Specifically, several typical applications based on the desired ceria nanostructures are focused to showcase the importance of nanostructure-derived effects. Moreover, some challenges and perspectives on the nanostructured ceria are presented, such as defects controlling and retainment, scale-up fabrication, and monolithic devices. Hopefully, this review can provide an improved understanding of nanostructured CeO_2 and offer new opportunities to promote the further research and applications in the future. DOI:10.1557/mrc.2016.52

Domain structures and magnetoelectric effects in multiferroic nanostructures

Deyang Chen and **Xingsen Gao**, South China Normal University, China; and **Jun-Ming Liu**, Nanjing University, China

Multiferroic nanostructures have been attracting tremendous attention not only for novel phenomena associated with fundamental physics, but also due to exciting application potentials in future nanoelectronic devices. In this mini-review, we first introduce several fabrication techniques recently developed for single phase and composite multiferroic nanostructures. Then, the topologic vortex domain structures in various ferroic nanostructures, which may bring about additional fundamental discoveries and applications in ultrahigh density recording, are discussed. Particular attention is paid to magnetoelectric effects in multiferroic nanodots, including room temperature electric field induced magnetic domain switching. Finally, existing challenges and new directions, e.g., cross-couplings among multiple functionalities, are prospected. We genuinely hope that this mini-review will arouse the readers' interest in this fascinating field. DOI:10.1557/mrc.2016.39

SPECIAL ISSUE RESEARCH LETTERS: FUNCTIONAL OXIDES

Solution-based synthesis of carbon–hematite composite thin films for high-performance supercapacitor applications

Jinzhan Su, **Shangpu Liu**, **Jian Wang**, **Cong Liu**, **Yufeng Li**, and **Dongyang Wu**, Xi'an Jiaotong University, China

Supercapacitor has received intense interest due to its high-charge/discharge rate and high-power density. C/Fe_2O_3 layer with different C/Fe ratios were synthesized by a solution-based approach for supercapacitor application. The influence of synthesis conditions on their electrochemical performances was investigated. Cobalt was added into C/Fe_2O_3 and significantly improved its performance. The optimal C/Fe_2O_3 sample gives a high specific capacitance of 85.3 F/g and the addition of Co_3O_4 further increase the capacitance of obtained C/Fe_2O_3/Co_3O_4 to 144.4 F/g at 5 A/g. This work demonstrates an efficient supercapacitor application of low-cost metal oxides and facile solution-based synthesis approach. DOI:10.1557/mrc.2016.60

Development of solution-processed nanowire composites for opto-electronics

David S. Ginley, National Renewable Energy Laboratory, USA; **Shruti Aggarwal**, Guru Gobind Singh Indraprastha University, India; **Rajiv Singh**, National Physical Laboratory, India; and **Tom Gennett**, **Maikel F. A.M. van Hest**, and **John D. Perkins**, National Renewable Energy Laboratory, USA

Silver nanowire-based contacts represent one of the major new directions in transparent contacts for opto-electronic devices with the added advantage that they can have ITO-like properties at

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substantially reduced processing temperatures and without the use of vacuum-based processing. However, nanowires alone often do not adhere well to the substrate or other film interfaces; even after a relatively high-temperature anneal and unencapsulated nanowires show environmental degradation at high temperature and humidity. Here we report on the development of ZnO/Ag-nanowire composites that have sheet resistance below 10 Ω/sq and >90% transmittance from a solution-based process with process temperatures below 200°C. These films have significant applications potential in photovoltaics and displays. DOI:10.1557/mrc.2016.49

Structure property relationships in gallium oxide thin films grown by pulsed laser deposition

Lauren M. Garten, **Andriy Zakutayev**, **John D. Perkins**, **Brian P. Gorman**, and **Paul F. Ndione**, National Renewable Energy Laboratory, USA; and **David S. Ginley**, Colorado School of Mines, USA

Beta-gallium oxide (β-Ga_2O_3) is of increasing interest to the optoelectronic community for transparent conductor and power electronic applications. Considerable variability exists in the literature on the growth and doping of Ga_2O_3 films, especially as a function of growth approach, temperature, and oxygen partial pressure. Here pulsed laser deposition (PLD) was used to grow high-quality β-Ga_2O_3 films on (0001) sapphire and (–201) Ga_2O_3 single crystals and to explore the growth, stability, and dopability of these films as function of temperature and oxygen partial pressure. There is a strong temperature dependence to the phase formation, morphology, and electronic properties of β-Ga_2O_3 from 350 to 550°C. DOI:10.1557/mrc.2016.50

Strain-induced modulation of oxygen vacancies and magnetic properties in $La_{0.5}Sr_{0.5}MnO_3$ thin films

Ji Ma, **Yujun Zhang**, and **Liang Wu**, Tsinghua University, China; **Chuangye Song**, Beijing Normal University, China; **Qinghua Zhang**, Tsinghua University, China; **Jinxing Zhang**, Beijing Normal University, China; and **Jing Ma** and **Ce-Wen Nan**, Tsinghua University, China

Oxygen vacancies have a significant impact on the structure and electrical/magnetic properties of doped manganites. Magnetic $La_{0.5}Sr_{0.5}MnO_3$ (LSMO) films were epitaxial grown on (001) $SrTiO_3$ substrate by pulsed laser deposition. Structural studies from the x-ray diffraction suggest that the as-grown films are fully constrained by the substrate with the thickness ranging from 8 to 40 nm. By examining the valence of Mn by x-ray photoelectron spectroscopy and x-ray absorption spectroscopy, we find the ratio of Mn^{4+}/Mn^{3+} increases along with the increased film thickness, which implies that the oxygen vacancies concentration induced by tensile strain correspondingly decreases. Therefore, the magnetization of LSMO is depressed with the exchange bias effect arising, and the electrical conductivity decreases significantly. This work builds a bridge between modulation of electric/magnetic properties and epitaxial strain in LSMO films. DOI:10.1557/mrc.2016.55

Tuning the physical properties of amorphous In–Zn–Sn–O thin films using combinatorial sputtering

P.F. Ndione and **A. Zakutayev**, National Renewable Energy Laboratory, USA; **M. Kumar**, Colorado School of Mines, USA; **C.E. Packard**, National Renewable Energy Laboratory and Colorado School of Mines, USA; **J.J. Berry** and **J.D. Perkins**, National Renewable Energy Laboratory, USA; and **D.S. Ginley**, Colorado School of Mines, USA

Transparent conductive oxides and amorphous oxide semiconductors are important materials for many modern technologies. Here, we explore the ternary indium zinc tin oxide (IZTO) using combinatorial synthesis and spatially resolved characterization. The electrical conductivity, work function, absorption onset, mechanical hardness, and elastic modulus of the optically transparent (>85%) amorphous IZTO thin films were found to be in the range of 10–2415 S/cm, 4.6–5.3 eV, 3.20–3.34 eV, 9.0–10.8 GPa, and 111–132 GPa, respectively, depending on the cation composition and the deposition conditions. This study enables control of IZTO performance over a broad range of cation compositions. DOI:10.1557/mrc.2016.57

PROSPECTIVE

Anodically grown functional oxide nanotubes and applications

B. Manmadha Rao, **Aida Torabi**, and **Oomman K. Varghese**, University of Houston, USA

Among various material nanoarchitectures, the nanotube geometry has received incredible attention due to the unique properties provided by its high surface area as well as nanoscale wall thickness and the availability of a variety of techniques to fabricate them. Since the beginning of this century, anodization has emerged as one of the most effective techniques for the fabrication of functional oxide nanotubes. Oxide nanotubes of a number of metals and alloys have been developed using this versatile technique. We review here the research activities on anodic nanotubes of various binary, ternary, and multinary materials and their selected applications. DOI:10.1557/mrc.2016.46

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RESEARCH LETTERS

Underlying causes of the magnetic behavior in surface patterned $NiFe_2O_4$ thin films

Goran Rasic and **Branislav Vlahovic**, North Carolina Central University, USA; and **Justin Schwartz**, North Carolina State University, USA

Surface patterned $NiFe_2O_4$ thin films exhibited large reduction in coercivity as compared with the films without surface patterning. Chemical analysis of the films revealed that there was no diffusion between the film and the substrate. Additional heating was shown to improve saturation magnetization without adverse effect on coercivity. The process of imprinting was eliminated as the possible cause of the phenomena as the flat stamp did not alter the magnetic properties of the film. Finally, it was shown that the orientation of the features with respect to the magnetic field does not have a significant effect on the magnetic response. DOI:10.1557/mrc.2016.38

"Green" electrospinning of a collagen/hydroxyapatite composite nanofibrous scaffold

David A. Castilla-Casadiego, **Michael Maldonado**, **Paul Sundaram**, and **Jorge Almodovar**, University of Puerto Rico Mayaguez, USA

In this work, a composite nanofibrous scaffold of collagen/hydroxyapatite was prepared by electrospinning using a mild solvent. Hydroxyapatite particles dispersed into a collagen/acetic acid/water solution was electrospun to yield composite nanofibers. Scanning electron microscopy reveals nanofibers with an average diameter of 342 ± 67 nm, and a rough surface caused by the hydroxyapatite particles. Both X-ray and infrared spectroscopy confirmed the presence of the hydroxyapatite particles embedded in the collagen fibers. The inclusion of hydroxyapatite particles does not alter the native collagen structure. Lastly, these composite nanofibers support pre-osteoblast adhesion. These results show how "green" electrospinning could be used to generate nanocomposite scaffolds with potential biomedical applications. DOI:10.1557/mrc.2016.43

X-ray reflectometry investigation of interfacial structure of CrAlN/TiAlN multilayers

Xiaoming Du, **Minpeng Wang**, and **Gang Zhang**, Shenyang Ligong University, China; and **Yan Wang**, **Xinxi Li**, and **Chaoqiang Huang**, China Academy of Engineering Physics, China

TiAlN, CrAlN films and alternate CrAlN/TiAlN multilayers with different repeated bilayer thickness ranging from 10 to 30 nm were prepared by reactive magnetron sputtering. The interface structures of the films were characterized using x-ray reflectometry method. The individual thickness of the repeated bilayers in multilayers and total thickness of the films are close to the nominal thickness and they are more accurate for thicker films. The interface roughness increases as the thickness of the repeated bilayer in mutilayers decreases. The scattering length density profiles of the films suggests that the chemical composition is more accurate for thicker films. DOI:10.1557/mrc.2016.44

Efficiency enhanced solar cells with a Cu_2O homojunction grown epitaxially on p-Cu_2O:Na sheets by electrochemical deposition

Tadatsugu Minami, **Jouji Yamazaki**, and **Toshihiro Miyata**, Kanazawa Institute of Technology, Japan

The Cu_2O homojunction was formed by epitaxially growing a manganese-doped Cu_2O (Cu_2O:Mn) thin film on thermally oxidized polycrystalline p-type sodium-doped Cu_2O (p-Cu_2O:Na) sheets by electrochemical deposition. A significant improvement of photovoltaic properties was achieved in solar cells fabricated by inserting a Cu_2O:Mn thin film between an Al-doped ZnO (AZO) transparent electrode and p-Cu_2O:Na sheets. The photovoltaic properties obtained in AZO/Cu_2O:Mn/p-Cu_2O:Na solar cells were controlled by changing the Mn content doped into the Cu_2O:Mn thin film. An efficiency of 4.21% was obtained in an AZO/Cu_2O:Mn/p-Cu_2O:Na solar cell fabricated with a Cu_2O:Mn thin film that was identified as an i-type semiconductor. DOI:10.1557/mrc.2016.45

Design of multi-layered TiO_2–Fe_2O_3 photoanodes for photoelectrochemical water splitting: patterning effects on photocurrent density

Myeongwhun Pyeon, University of Cologne, Germany; **Meng Wang**, University of Cologne, Germany and Xi'an Jiaotong University, China; **Yakup Gönüllü** and **Ali Kaouk**, University of Cologne, Germany; **Sara Jäckle** and **Silke Christiansen**, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH and Max Planck Institute for the Science of Light, Germany; **Taejin Hwang** and **Kyoungll Moon**, Korea Institute of Industrial Technology, South Korea; and **Sanjay Mathur**, University of Cologne, Germany

We report the effect of patterning on photoelectrochemical (PEC) water-splitting performance. Oxide–oxide heterostructures based on horizontal and vertical heterojunctions were fabricated on transparent conductive oxide glass by sequential plasma enhanced chemical vapor deposition (PECVD) of individual metal oxide. Featured masks were employed to enable

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three-dimensional patternings of stripes and cross-bars structures formed by Fe_2O_3 and TiO_2 layers. PEC measurement was carried out by a three-electrode cell. It was found that double layered TiO_2//Fe_2O_3:FTO showed a decrease in PEC performance when compared with single Fe_2O_3:FTO layer, whereas triple-layered Fe_2O_3//TiO_2//Fe_2O_3:FTO (both patterned and unpatterned samples) displayed enhanced photocurrent density. The results show that the existence of multiple phase boundaries does not always add up to PEC enhancement observed in single heterojunction. DOI:10.1557/mrc.2016.54

Growth process and morphology control of SBA-15 particles: synergistic effects of tetraethoxysilane and Pluronic-123 concentrations

Kai Zhuang, **Guangfu Yin**, **Ximing Pu**, **Xianchun Chen**, **Xiaoming Liao**, **Zhongbin Huang**, and **Yadong Yao**, Sichuan University, Chengdu, China

The synergistic effects of the template [Pluronic-123 (P123)] and the silica source [tetraethoxysilane (TEOS)] concentrations on the SBA-15 mesoporous silica morphology were investigated through adjusting the system initial solution volume with the same amounts of silica source and template. It found interestingly that the SBA-15 morphology changed from the hexagonal plate-like shape to the gear-like shape with the decrease of the P123 and TEOS concentration. Based on the morphology variations, the growth of the gear-like morphology was speculated to be formed through the preferential growth at the corner and the layer-by-layer growth in the end face of the ordinary hexagonal plate-like particle. DOI:10.1557/mrc.2016.56

Grain boundary stability and influence on ionic conductivity in a disordered perovskite—a first-principles investigation of lithium lanthanum titanate

Kathleen C. Alexander, Massachusetts Institute of Technology, USA; and **P. Ganesh**, **Miaofang Chi**, **Paul Kent**, and **Bobby G. Sumpter**, Oak Ridge National Laboratory, USA

The origin of ionic conductivity in bulk lithium lanthanum titanate, a promising solid electrolyte for Li-ion batteries, has long been under debate, with experiments showing lower conductivity than predictions. Using first-principles-based calculations, we find that experimentally observed type I boundaries are more stable compared with the type II grain boundaries, consistent with their observed relative abundance. Grain boundary stability appears to strongly anti-correlate with the field strength as well as the spatial extent of the space charge region. Ion migration is faster along type II grain boundaries than across, consistent with recent experiments of increased conductivity when type II densities were increased. DOI:10.1557/mrc.2016.58

Enhanced mechanical properties of machinable mica glass ceramics at cryogenic temperatures

Juan Chen and **Zhipeng Xie**, Tsinghua University, China

Machinable mica glass ceramics were synthesized by sintering method. The crystal phase was characterized using x-ray diffraction, showing that the main crystal phase was fluorophlogopite. Mechanical properties were measured at different temperatures. The results demonstrated that bending strength and fracture toughness increased 28% and 24% when temperature decreased from 300 to 77 K, respectively. Compressive strength also increased at cryogenic temperatures, but a higher value was obtained at 195 K. According to scanning electron microscope observation, the extraction of mica platelets was observed at 77 K, which may be the toughening mechanism of machinable mica glass ceramics. DOI:10.1557/mrc.2016.59

Enhancement of dielectric properties with the addition of bromine and dopamine modified barium titanate particles to silicone rubber

Liang Jiang, **David Kennedy**, **Stephen Jerrams**, and **Anthony Betts**, Dublin Institute of Technology, Ireland

Dual-coated barium titanate (BT) particles were prepared using dopamine (DP) in conjunction with bromine (Br) in order to enhance the dielectric constant of silicone rubber (SR) composites containing evenly distributed BT particles. The results showed that both DP and Br were deposited on the BT particles. The dielectric constant of the SR/BT composite was significantly increased from 3.6 to 4.7 at 1 kHz with the addition of BT modified with dopamine (DP–BT). Moreover, the dielectric constant further rose to 4.9 at 1 kHz when the DP–BT particle was grafted with bromine (Br–DP–BT). DOI:10.1557/mrc.2016.53

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