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ABSTRACT BOOK

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Introduction

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How to Use the Abstract Book

Refer to the Table of Contents to determine page numbers on which specific session abstracts begin. At the beginning of each session are headings that list session title, location and session chair. Starting times for presentations and paper numbers precede each paper title. The Author Index lists each author and the page number on which their abstract can be found.

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Wednesday, January 18, 2017

Plenary I

Room: Indian

Session Chair: Geoff Brennecke, Colorado School of Mines

8:40 AM

(EMA-PLEN- 001-2017) Thermochemistry of Redox Active Oxides and its Relevance to Solar Fuel Generation

S. Haile^{*1}; 1. Northwestern University, USA

Laboratories around the world are pursuing a variety of promising strategies for converting solar energy into a reliable energy source for on-demand utilization. We describe here a thermochemical approach for achieving this goal using solar heat as the energy source and redox active non-stoichiometric oxides as the reaction medium. Specifically, upon exposure to high temperatures and/or inert gas, the oxide undergoes reduction (without change in crystalline phase) to release oxygen. Upon exposure to H₂O (or CO₂), the oxide is reoxidized, releasing H₂ (or CO). We compare the thermochemical fuel production behavior of a variety of oxides, including those of the fluorite structure-type (ceria and its derivatives) and those of the perovskite structure-type (La_{1-x}Sr_xMnO₃). A shared characteristic of the most promising materials is that bulk oxygen diffusion (chemical diffusion) is fast such that fuel production rates are limited either by surface reaction kinetics or, at high temperatures, gas-phase mass transfer rates. We develop an analytical model to treat the behavior under gas-phase limited behavior and explore the implications on fuel production rates.

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Material Design, Fabrication and Applications I

Room: Indian

Session Chairs: Satoshi Wada, University of Yamanashi;

Dragan Damjanovic, Swiss Federal Institute of Technology in Lausanne

10:00 AM

(EMA-S1-001-2017) Can conductivity have beneficial effect on electro-mechanical response? (Invited)

T. Rojac²; D. Damjanovic^{*1}; 1. Swiss Federal Institute of Technology in Lausanne, Switzerland; 2. Jozef Stefan Institute, Slovenia

The electrical conductivity (ac or dc) is usually considered as detrimental to electro-mechanical properties of ferroelectrics: for example, samples with elevated conductivity are usually considered to be difficult to polarize and conductivity is one factor responsible for charge drifts in sensors. In materials in which mechanical and electrical properties are coupled, conductivity affects mechanical properties and vice versa. Mechanical losses in a piezoelectric resonator may thus be influenced by electrical conductivity of the sample. Charge transport within heterogeneous samples affects local fields and contributes strongly to the piezoelectric (or in general, electro-mechanical) properties, leading to the piezoelectric Maxwell-Wagner effect. Interesting situation arises when conductive paths are ferroelastic domain walls. Both stationary and moving domain walls are known to be strong contributors to the piezoelectric properties. Electrically conductive domain walls contribute to the piezoelectricity in a fashion very different from nonconducting domain walls. We will present evidence that the same defects that control bulk conductivity may control conductivity of domain walls. We shall discuss in detail the case of BiFeO₃ where atomic defect

structure is essentially different than in perovskite titanates especially after annealing in reducing, inert or oxidizing atmospheres.

10:30 AM

(EMA-S1-002-2017) Preparation of New Barium Titanate-based Nano-complex Ceramics with High-density Heteroepitaxial Interfaces by Solvothermal Solidification Method and Their Dielectric and Piezoelectric Enhancement (Invited)

S. Wada^{*1}; 1. University of Yamanashi, Japan

These nano-complex ceramics prepared in this study were porous with a porosity of around 25 ~ 35 %. The dielectric measurements showed that for the BT-KN nano-structured ceramics with KN/BT ratio of 1, the dielectric constant was 300 at 20°C and 1 MHz, while for the BT-BF nano-complex ceramics with BF/BT ratio of 1, the dielectric constant was 70 at 20°C and 1 MHz. The strain vs. electric-field curves were also measured for these ceramics, and it was found that the apparent d_{33}^* estimated from its slope of the strain vs. electric-field curves was almost 100 pm/V for the BT-KN nano-complex ceramics, while the apparent d_{33}^* for the BT-BF nano-complex ceramics was less than 20 pm/V. To explain the results, we proposed structure-gradient region (SGR) model dependent of lattice mismatch and material hardness.

11:00 AM

(EMA-S1-003-2017) Thick Film Dielectrics Produced via Aerosol Deposition

E. Patterson^{*1}; E. Gorzkowski¹; S. D. Johnson¹; 1. Naval Research Lab, USA

Aerosol deposition (AD) is a thick-film deposition process that can produce layers up to several hundred micrometers thick with densities greater than 95% of the bulk. The primary advantage of AD is that the deposition takes place entirely at ambient temperature; thereby enabling film growth in material systems with disparate melting temperatures. The bonding and densification of the film and film/substrate interface are thought to be facilitated by local temperature rise, high pressure, and chemical bonding during deposition, which leads to a dense nano-grained microstructure. In this talk we present results on the deposition of dielectric and ferroelectric materials deposited by aerosol deposition including the effect of processing parameters on the resultant material properties.

11:15 AM

(EMA-S1-004-2017) Physical properties of methylammonium lead iodide prepared via a bulk synthesis route

W. L. Schmidt^{*1}; J. Passarelli¹; C. D. Kennedy¹; H. Chen¹; D. C. Sinclair¹; I. M. Reaney¹; 1. The University of Sheffield, United Kingdom

Organometal halide perovskites have dramatically changed the focus of solar cell research in the past few years. Various compositions have been used in a range of solar cell geometries to reach efficiencies in excess of 20%. Pure CH₃NH₃PbI₃ (MALI) is no longer the preferred material for implementation into solar cells due to its instability during operation and the difficulties of consistent scalable processing. However, bulk preparation of MALI is desirable to provide a generic, high purity feedstock for further compositional modification. In this work a standard ball milling method is used to create bulk powders of MALI to understand the compositional effect on the material properties such as thermal conductivity, electrical conductivity, permittivity, thermal stability and degradation. Production of the powder is easily scaled up to 50g batches with consistent material properties. Comparison with other preparation routes will be made.

11:30 AM

(EMA-S1-005-2017) Synthesis of High Surface Area Molybdenum Carbide as a Catalyst

S. Nayak^{*1}; A. Benavidez¹; F. Garzon²; 1. University of New Mexico, USA; 2. University of New Mexico/ Sandia National Laboratories, USA

The electrochemical synthesis of ammonia may be considered as a possible viable alternative to the conventional Haber-Bosch process. However, high surface area electrocatalysts need to be developed for the process. Molybdenum nitride may be considered as a suitable electrochemical catalyst because of its electrical conductivity and catalytic activity towards ammonia formation. However, in the presence of air, Mo₃N gets deactivated due to the formation of oxy-nitride. In order to overcome catalyst deactivation, molybdenum carbide may be a good substitute candidate for the electrocatalyst in this process. In this study, we are using an ion exchange method to synthesize molybdenum carbide. The synthesis process involves exchanging a resin with an ammonium molybdate precursor followed by carbonizing it in argon or nitrogen at temperatures between 800°C and 1000°C. By varying the synthesis conditions, we have formed both a cubic phase MoC and a mixture of cubic MoC and hexagonal Mo₂C. The XRD and HRTEM analysis shows nanoparticles of around and less than 5 nm. However, the BET surface area of the carbides is low (~ 6 m²/g) due to the excess amorphous carbon surrounding the crystallites. We are exploring methods to remove the excess carbon via the methane formation reaction.

11:45 AM

(EMA-S1-006-2017) Nickel oxide doped barium yttrium zirconate nanostructures

I. Reimanis^{*1}; A. Morrissey²; J. R. O'Brien³; 1. Colorado School of Mines, USA; 2. CoorsTek, Inc., USA; 3. Off Grid Research, USA

The design of high surface area, nanostructured metal-ceramic systems is important for a wide range of energy related applications, including catalysts, fuel cells, and ionic transport membranes. Yttrium doped barium zirconate (BZY) is an important material in this realm, and when doped with nickel oxide, and subsequently exposed to reducing conditions, some very interesting nanostructures form. In the present work SQUID magnetometry and transmission electron microscopy is used to describe these structures. It is shown that the nickel-oxide doped BZY may be designed so that a shell structure protects barium volatilization during high temperature exposure, and that it ultimately leads to a barium nickel oxide phase that is selectively reduced to nickel metal. The resulting material should exhibit superb catalytic reactivity.

12:00 PM

(EMA-S1-007-2017) Densification of fragile ferroic phases through high pressure low temperature spark plasma sintering (SPS)

T. Herisson de Beauvoir^{*1}; U. Chung Seu¹; F. Molinari¹; M. Josse¹; 1. ICMCB-CNRS, France

For many applications, densification is a key point which condition the development of devices from functional materials. It's the case for ferroic and multiferroic materials on which we have to deposit electrodes for the specific measurement of their dielectric properties. Looking for possibly multiferroic phases lead us to consider a wide range of materials exhibiting interesting crystal structures and compositions for potential ferroic properties. The common point of these materials is the difficulty to access high densification level (> 90% compactness) necessary for reliable dielectric characterizations. Spark plasma sintering (SPS) was mostly used up to now to sinter materials under high temperatures with fast ramp, applying mostly low pressures (often up to 100MPa). We got interested in some materials having low decomposition temperatures (typically <700°C) preventing them from being sintered under classical conditions. Up to now, not only did we managed to sinter what we call

"fragile" phases, but we also were able to stabilize some phases at much higher temperatures than their stability in air. We used the obtained ceramics to perform dielectric measurements within a PPMS, enabling the application of magnetic field during dielectric measurement to investigate the magnetoelectric response of our samples.

12:15 PM

(EMA-S1-008-2017) Chemical solution deposition of orthorhombic/tetragonal phase hafnium oxide

W. Straka^{*1}; J. Schwartz¹; 1. North Carolina State University, USA

Hafnium oxide has a high dielectric constant which makes this material useful to replace SiO₂ as a high-k dielectric material. Additionally, a few orthorhombic phases of this material have recently been discovered that are ferroelectric. As a result, there has been much research effort into the non-monoclinic phases of hafnia in thin film form. The majority of the synthesis routes for these phases are from vacuum based deposition techniques which are costly and difficult to scale. Using chemical solution deposition (CSD), the tetragonal/orthorhombic phase of hafnia can be made. The processing parameters that affect phase and grain structure will be highlighted. The films are characterized through x-ray diffraction and microscopy techniques. Their electrical properties will also be shown.

S2: Advanced Processing for Electronic and Electrochemical Systems: Crystals, Films and Devices

Refined Synthesis Routes to Advance and Enable Properties I

Room: Coral B

Session Chair: Elizabeth Paisley, Sandia National Laboratories

10:00 AM

(EMA-S2-001-2017) New Routes for Designing Next Generation Dielectrics and Capacitors (Invited)

C. Randall^{*1}; D. S. Heidary¹; L. Gao¹; J. Guo²; H. Guo¹; S. Dixit³; R. Dixit³; A. Baker¹; 1. Penn State University, USA; 2. The Pennsylvania State University, USA; 3. DRS Research, USA

Capacitors and dielectric materials need to be considered for future opportunities. That will require higher energy densities, higher breakdown strengths, and broad thermal stability. In this presentation, we will review the materials of choice that are under development. We will also introduce some novel ideas in regard to expanding the processing strategies to manufacture next generation multilayer ceramic capacitors. These new techniques include thermal plasma spray, firing base metal multilayers at high partial pressure of oxygen, and exploring low temperature cofiring of multilayers. Acknowledgements: DRS Research subaward no. 165167, prime award no. DE-SC0010164 (U.S. Dept. of Energy) National Science Foundation, as part of the Center for Dielectrics and Piezoelectrics under Grant Nos. IIP-1361571 and 1361503

10:30 AM

(EMA-S2-002-2017) Hydrothermal sintering at near room temperature (Invited)

X. Kang^{*1}; R. Floyd¹; E. C. Dickey¹; C. Randall²; J. Maria¹; 1. North Carolina State University, USA; 2. Pennsylvania State University, USA

Traditional solid state densification process of ceramics requires a high thermal budget for bulk diffusion with temperature routinely well above 1000°C. Such high fabrication temperature imposes great limitation on material selection due to thermal incompatibility issues, such as de-wetting of metal contacts, thermal stress induced by thermal expansion mismatch and high temperature volatility and

oxidation. It also has a huge impact on energy consumption and the environment. The recent discovery of water assisted densification of Li_2MoO_4 at room temperature potentially could be a solution to these problems however the underlying mechanism is not yet fully understood. In this talk near complete densification of Li_2MoO_4 and ZnO at temperatures around 100°C is demonstrated in a one-step uniaxial consolidation process. Effects of individual process parameter, such as temperature, pressure and properties of solution added, etc. are discussed and the underlying densification mechanisms are deduced. From studying densification characteristics of chemically dissimilar materials, favorable characters of material systems are proposed and application of this concept to a wide selection of materials is discussed.

11:00 AM

(EMA-S2-003-2017) Electrical properties and applications of pressure-assisted hydrothermal densified (PAHD) ZnO

R. Floyd^{*1}; X. Kang¹; J. Maria¹; 1. North Carolina State University, USA

Substantial densification can be promoted by mixing an oxide with a liquid phase – provided some finite solubility of the two – and uniaxially pressing and heating the die. We refer to this process as Pressure-Assisted Hydrothermal Densification (PAHD) due to the combination of modest temperature and high pressure. ZnO powders can be reproducibly densified in pellet form to >99%. PAHD creates a new pathway for introducing dopants into the grain boundaries, thereby affecting the electrical properties of the resulting polycrystal. In this presentation we present results from a series of PAHD experiments where intrinsic and traditionally doped ZnO powders were mixed with liquid phases containing a variety of aliovalent dopants. Conductivity and dielectric properties were measured and compared to traditionally sintered samples. We observe that donor doped ZnO powders produce insulating polycrystals when the liquid phase contains no donors. We interpret this result based on differential solubility of cations during the densification stage and the production of pure ZnO grain boundaries. When donors such as Al are introduced into the liquid, finite conductivity can be observed. This work shows potential applications of PAHD for ultra-low temperature synthesis of electronic components, such as ZnO varistors where electronic function can be engineered through the densification method.

11:15 AM

(EMA-S2-004-2017) Processing and properties of transparent anisotropic ceramics (Invited)

A. Dupuy²; A. Wieg²; E. Penilla²; Y. Kodera²; J. E. Garay^{*1}; 1. UC San Diego, USA; 2. UC Riverside, USA

Light scattering due to birefringence has prevented the use of polycrystalline ceramics with anisotropic optical properties in applications such as laser gain media. However, continued development of processing technology has allowed for very low porosity and fine grains, significantly improving transparency and is paving the way for polycrystalline ceramics to be used in demanding optical applications. We will discuss the important microstructural features that contribute to the optical properties and some processing techniques that allow for microstructural control. Specifically, we will discuss the role of point defects as purposely added dopants and unwanted contaminants as well as secondary phases in oxides and nitrides. We will also show results from on going efforts to develop ceramics for light emitting (photoluminescence) and light controlling (electro-optic) applications. An important theme for the electro-optic work is developing powder formulations that allow one to lower densification temperatures. In the photoluminescence case we discuss the role of dopant concentrations and dopant agglomeration on the optical properties.

11:45 AM

(EMA-S2-005-2017) Flash sintering of thorium dioxide

W. Straka^{*1}; J. Schwartz¹; 1. North Carolina State University, USA

Thorium dioxide is a binary oxide that has applications as a refractory ceramic and as a nuclear fuel. This material has advantages over uranium-based nuclear fuels due to its higher burn-up, higher energy density, wider availability, and nuclear non-proliferation. However, this material has the highest melting point of any known binary oxide at 3400°C . Overcoming these thermodynamic boundaries has historically been overcome through dopants and reduction in grain size. Using a fairly new ceramic processing technique, flash sintering, this material has been found to densify to about 95 % dense at about 950°C . The effects of electric field magnitude and current magnitude are reported. Electron microscopy images show little effect on the grain size and will be shown.

12:00 PM

(EMA-S2-006-2017) Use of oriented 2-dimensional BN ceramic arrays to achieve controllable bandgap for tunable electronics

M. Rivera¹; R. Velazquez¹; P. Feng^{*1}; 1. UPR, USA

Our work is to understand tunable bandgap structures of low dimensional (LD) wide bandgap boron nitride (BN) ceramic materials for developing zero power, tunable electronic devices for extreme environment. Use of controllable orientations and edge structures is the soul of present study to control bandgap structures. This is very different from traditional doping or plasma or chemical surface treatments for manipulation of the bandgap. Because the system completely avoids doping and impurity, possibility of impure diffusion is eliminated. As a result, the newly designed and fabricated electronic devices perform extremely well at wide range of temperatures, making it particularly important applications in harsh environments.

S5: Energy Sustainable Optoelectronics and Magnetoelectronics

Materials for Optoelectronics and Electro-Optics I

Room: Mediterranean C

Session Chairs: Jian Shi, Rensselaer Polytechnic Institute;

Jennifer Andrew, University of Florida

10:00 AM

(EMA-S5-001-2017) Advanced metrology for early-stage photovoltaic materials: Transient THz photoconductivity measurements of minority-carrier lifetime in tin sulfide (Invited)

R. Jaramillo^{*1}; M. Sher²; B. Ofori-Okai¹; V. Steinmann¹; C. Yang³; K. Hartman¹; K. Nelson¹; A. Lindenberg⁴; R. Gordon³; T. Buonassisi¹; 1. Massachusetts Institute of Technology, USA; 2. Wesleyan University, USA; 3. Harvard University, USA; 4. Stanford University, USA

Minority carrier dynamics is at the core of photovoltaic (PV) operation. Screening materials based on minority carrier dynamics is an attractive strategy to discover new semiconductors for PV. Unfortunately, extracting relevant information from less-studied materials is challenging, even with state-of-the-art techniques. Here we measure bulk and surface minority carrier recombination in SnS thin films. SnS has manufacturing advantages for thin film PV and has seen recent efficiency gains, including a record 4.36% (certified) efficient device. The bulk minority carrier lifetime (τ) is below 100 ps in the record devices. Modeling suggests that efficiencies of 10% or more could be achieved with τ on the order of 1 ns. We measure transient photoconductivity in an optical-pump, THz-probe configuration. We model our data with diffusive dynamics and perform global fits over large data sets to increase confidence in our fitted parameters. We use these measurements to inform defect engineering techniques including annealing and surface oxidation.

Our results illustrate the challenges of measuring non-equilibrium dynamics in new materials, and point to processing steps that may improve solar cell efficiencies.

10:30 AM

(EMA-S5-002-2017) Hybrid Perovskite Photodetectors (Invited)

T. Wu^{*1}; 1. KAUST, Saudi Arabia

Rediscovery of hybrid perovskites, such as $\text{CH}_3\text{NH}_3\text{PbX}_3$, where X is Cl, Br or I, in high-performance photovoltaic research has aroused lots of interest from the materials science community. Their exceptional properties, such as low-cost solution processing, tunable direct bandgap, high light absorption and long carrier diffusion length, might lead to paradigm-shifting technologies in the near future. I will discuss the perspective of applying hybrid perovskites in photovoltaic and optoelectronic devices, with a focus on photodetectors and phototransistors. Our experiments on perovskite phototransistors provided direct evidence on the ambipolar transport in perovskite films with balanced electron and hole mobilities. As an approach towards high-mobility devices, we found that carbon nanotubes embedded in perovskite films can serve as one-dimensional transport channels and significantly enhance the charge mobility to a level comparable to common semiconductors such as crystalline silicon. Furthermore, two-dimensional metal dichalcogenides were used to boost the performance of perovskite-based photodetectors. Finally, I will discuss the application of perovskite microcrystal films as photodetectors that operate efficiently in both broadband and narrowband regimes.

11:00 AM

(EMA-S5-003-2017) Nanostructured Organometal Halide Perovskites for Light Emitting Diodes (Invited)

B. Ma^{*1}; 1. Florida State University, USA

Organometal halide perovskites, an emerging class of solution processable organic-inorganic hybrid materials, have attracted great attention for their applications in optoelectronic devices. Provided the high color purity and tunability, organometal halide perovskites are promising light emitters. However, the overall performance of perovskite based LEDs reported to date has not reached to the levels of typical organic and quantum dot LEDs yet, in part due to the low photoluminescence quantum yields of bulk perovskites. In this talk, I will present our recent efforts on developing highly luminescent nano/micro-scale organometal halide perovskites, and discuss their application in efficient LEDs. Color tuning by quantum size confinement can be achieved for nanoscale perovskites with a chemical formula of $(\text{RNH}_3)_2(\text{CH}_3\text{NH}_3)_{n-1}\text{Pb}_n\text{Br}_{3n+1}$. By synthetic control of n, from one to various defined integer numbers and infinite, 2D, quasi-2D, and 3D structures with tunable emission colors can be obtained. Besides perovskites with narrow emissions, we have also developed microcrystalline perovskites with broadband emission across the entire visible spectrum, which can be used as a single component phosphor for down conversion white LEDs.

11:30 AM

(EMA-S5-004-2017) CdTe thin film solar cells: Bandgap Engineering via alloying (Invited)

F. Yan^{*1}; 1. First Solar, USA

CdTe thin-films are today's dominant thin-film technology in the photovoltaic industry. Efficiency of thin-film CdTe solar cells have increased from 16% a few years ago to 22%, now surpassing the market dominant multi-crystalline Si technology. Several technology components have contributed to the sudden rise of efficiency, one of them is to effectively grade the solar-cell absorber band-gap. Historically, alloying was limited by the miscibility gap of the CdS-CdTe system, more recently we have found that the CdSe-CdTe system provides greater opportunity. In this talk, we present work that investigated additional external dopants to further engineer the bandgap in CdSeTe via alloying. It is demonstrated that

various dopants can be applied to narrow the bandgap of CdTe devices as it is observed in a crystalline or thin-film form. Initial device results can confirm a red-shift of the absorption edge in the spectral response, however, are overall poor due to the complexity of integration into the downstream process flow. Overcoming these integration problems may enable further performance gain for CdTe thin-film PV devices.

12:00 PM

(EMA-S5-005-2017) Halide Perovskites for Light Emitting Diodes (Invited)

H. Gao^{*1}; 1. Florida State University, USA

Solution-processed halide perovskites have shown their promises in a variety of optoelectronic applications, from solar cells, light emitting diodes, to photodetectors. This new class of optoelectronic materials exhibit superb optical and electrical properties such as long diffusion length, high carrier mobility, strong optical absorption, and tunable bandgap. Despite the successful demonstrations reported so far, perovskite-based devices with high performance and stability still remain challenging. Our work has been focused on creating halide perovskites for electrically-driven LEDs. We found that the morphology of the materials, either nanostructured or microcrystalline, plays important role in both optical and electrical properties. With optimized morphology, perovskite-based LEDs with high brightness and external quantum efficiencies have been achieved. The approaches to control and manipulate crystallization of halide perovskite may also be applicable to the development of other optoelectronic applications such as solar cells.

S9: Interfaces in Microstructural Evolution: Structure, Properties, Anisotropy, and Motion

Grain Growth: Impact of Anisotropy and Other Interfacial Properties

Room: Mediterranean A/B

Session Chairs: John Blendell, Purdue University;

Wolfgang Rheinheimer, Karlsruhe Institute of Technology

10:00 AM

(EMA-S9-001-2017) The Five-Parameter Grain Boundary Curvature Distribution in Strontium Titanate (Invited)

X. Zhong¹; M. N. Kelly²; G. Rohrer^{*1}; 1. Carnegie Mellon University, USA

A method is described that can be used to measure the distribution of grain boundary curvatures as a function of five independent crystallographic parameters. For validation, the method is tested on ideal shapes and it is shown that for appropriate resolution and reconstruction procedures, accurate curvatures can be measured. The method is also applied to three-dimensional microstructure data for strontium titanate. It is found that the grain boundary mean curvature varies with the boundary crystallography and is more sensitive to the grain boundary plane orientation than to the disorientation. The grain boundaries with the smallest curvatures also have low grain boundary energy and large relative areas.

10:30 AM

(EMA-S9-003-2017) An explanation for the maintenance of the polyhedral shape of abnormal grains during their growth (Invited)

S. L. Kang^{*1}; S. Jung²; 1. Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea; 2. Agency for Defence Development, Republic of Korea

In many single phase systems, such as BaTiO_3 and Ni, the shape of abnormal grains is well faceted and is maintained during their growth. It was puzzling that the velocity of the faceted migrating

boundary of the abnormal grains is constant, irrespective of the orientations of the adjacent shrinking grains. To understand the shape maintenance of abnormal grains, we carefully observed the migrating and impinged boundaries of abnormal grains in a model Ni system. We found that the grain boundaries terminated by {100} planes were singular with atomic steps and have a lower energy than the boundaries terminated by other planes. These findings indicate that grain growth in Ni is governed by the movement of {100} singular planes, i.e., the step formation and spreading at the singular planes, similar to the migration of a faceted solid/liquid interface. The results are also discussed in relation to previous experimental observations in other systems.

11:00 AM

(EMA-S9-004-2017) Faceted Grain Growth in the NiO-MgO System

D. Lowing^{*1}; J. Blendell¹; 1. Purdue University, USA

The effect of anisotropic grain boundary energy on grain growth and grain boundary morphology is studied using the NiO-MgO system. NiO-MgO in an isomorphous system with complete solid solubility that has a large change in the faceting behavior with composition, changing from (100) dominated to (111) dominated. Homogeneous powders were prepared using a citrate route, however poor densification resulted in porous microstructures. Hot pressing or SPS in reducing atmosphere resulted in Ni metal precipitation and inhomogeneities. To overcome this problem, grain growth studies were carried out on fully dense agglomerates over a range of temperatures using three compositions of NiO-MgO. The effect of composition on grain growth rate was measured. It is postulated that the effect is due to the changing grain boundary structure of the polycrystal as the anisotropy of the energy changes. The effect was strongest at higher temperatures.

11:15 AM

(EMA-S9-005-2017) Grain growth transitions in Barium Strontium Titanate

F. J. Altermann^{*1}; W. Rheinheimer¹; M. J. Hoffmann¹; 1. Karlsruhe Institute of Technology, Germany

Barium titanate and strontium titanate were used as model systems to study grain growth in perovskites. In both materials a grain growth anomaly was found: In the case of barium titanate grain growth shows a transition to faster growth with increasing temperature whereas strontium titanate indicates a transition region with exponentially reduced grain growth with increasing temperature. In both materials the transitions are strongly correlated to abnormal grain growth. Since barium titanate and strontium titanate show perfect miscibility, grain growth experiments on barium strontium titanate were used to reveal the relationship between these two effects. It is shown that grain growth rates and bimodality of the microstructures are a function of the Ba/Sr ratio and a close relation to the point defect chemistry of the perovskites can be found. The counterintuitive behaviour of (Ba,Sr)TiO₃ is discussed in relation to the grain boundary mobility and energy and an explanation for the grain growth transitions based on grain boundary characteristics and defect distribution is presented.

11:30 AM

(EMA-S9-006-2017) Grain growth in perovskites: Observation and modelling of bimodal microstructure evolution

W. Rheinheimer^{*1}; E. Schoof¹; M. Selzer¹; B. Nestler¹; M. J. Hoffmann¹; 1. Karlsruhe Institute of Technology, Germany

Several perovskite ceramics are known to show non-Arrhenius grain growth. In particular for strontium titanate a grain growth transition was documented with decreasing grain growth rates with increasing temperature. Other materials as barium titanate, lithium lanthanum titanate and barium strontium titanate indicate grain growth transitions as well. The growth transitions are coupled to bimodal

microstructures and seem to be caused by the existence, coexistence and transition of different grain boundary types. This talk gives a review on the details of the grain growth transitions in perovskites. A simple mean field approach and standard grain growth experiments are compared with phase-field simulations of grain growth. Important parameters such as atomistic boundary structure, segregation effects, wetting transitions, faceting, grain boundary stoichiometry, space charge and interfacial drag effects are discussed with respect to their impact on grain growth in perovskites. A summary of open questions and future directions is given.

11:45 AM

(EMA-S9-007-2017) Application of Minkowski Hull to Ceramics Intergranular Phenomena

V. Mitic^{*1}; L. Kocic¹; V. Paunovic¹; 1. University of Nis, Serbia

Intergranular contacts in materials obtained by powder processing technologies are responsible for many characteristics of this material from mechanical to electric or optical. Special importance of such inter-grain contacts is emphasized in sintered ceramics, due to characteristic role of liquid sintering phase. It is helpful to introduce a 3D object formed by a convex body moving around the grain, an object known as the Minkowski hull (MH). Here, some properties of MH are studied and some applications are suggested. The whole construction leads to a natural generalization which makes possibility of introducing fractal forms, which, in fact are in capacity to realistically describe the surface of the grains. This concept is very useful in defining the measure of closeness between two or more grains from disjoint hulls to stable three-point grains' contact. In combination with space configuration of grains' network such closeness measure the fractal configuration of intergranular contacts of different thickness is modeled. It causes many versatile micro-electronic situations that implies corresponding material behavior. Using generalized Minkowski hull, the extreme situations: contact – no contact are refined to several sub-situations that then explain some details connected to micro-capacities, thermodynamics, ferro-electric etc.

S12: 5G Materials for the Millimeter Wave Revolution

5G Materials for the Millimeter Wave Revolution I

Room: Caribbean B

Session Chair: Nate Orloff, NIST

10:00 AM

(EMA-S12-001-2017) Enhanced Materials in Bulk Acoustic Wave Filters for 4G and 5G Wireless (Invited)

J. Sadhu^{*1}; J. Modarres¹; M. Wang¹; F. Dumont¹; R. Kraft¹; 1. Qorvo, USA

The burgeoning demand for wireless connectivity of mobile devices and the emerging Internet of Things (IoT) places critical challenge on the usage of the RF spectrum bands needed to carry this data. Avoiding complex interference challenges between closely spaced bands remains a key consideration for 4G-LTE smartphones and the issue will only be compounded as more spectrum bands proliferate in 5G. Today, the stringent demands of RF filtering are met by highly selective bulk acoustic wave (BAW) filters. The demand for the number of BAW filters in mobile devices have quadrupled in the past two years and is expected to rise with 5G. At the same time, BAW filter technology faces challenges to provide low-loss, wide bandwidth filters with high out-of-band isolation. In this paper, we discuss the improvements in the piezoelectric thin films employed in BAW filters. Next-generation materials need disruptive enhancement in piezoelectric response over traditional aluminum nitride (AlN), specifically electromechanical coupling (kt₂). Enhancing coupling results in higher bandwidth and/or better insertion loss at band edges. Substituting transition metal elements like scandium

into AlN films enables up to 50% increase in κt_2 at only ~10% Sc. We also provide case studies of bands wherein better rejection & wider bandwidth with enhanced κt_2 improves multiplexing of these bands and allows carrier aggregation.

10:30 AM

(EMA-S12-002-2017) Designer $(\text{SrTiO}_3)_n(\text{BaTiO}_3)_m\text{SrO}$ Superlattices for mmWave Tunable Dielectrics (Invited)

N. M. Dawley^{*1,4}; X. Lu¹; N. Orloff¹; M. E. Holtz²; C. Lee⁴; J. Zhang³; D. A. Muller²; J. C. Booth¹; D. G. Schlom⁴; 1. NIST, USA; 2. Cornell University, USA; 3. Massachusetts Institute of Technology, USA; 4. Cornell University, USA

At gigahertz frequencies, the thin-film tunable dielectric material, $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$, experiences large dielectric loss, attributed to non-stoichiometric point defects. We use oxide molecular-beam epitaxy (MBE) as a controlled way to fabricate the next generation of thin-film, mmWave tunable dielectrics via precise atomic layering and epitaxial strain. Using this approach we recently demonstrated record tunable dielectric performance at gigahertz frequencies for strained $(\text{SrTiO}_3)_n\text{SrO}$ Ruddlesden-Popper (RP) phases through the accommodation of point defects by $(\text{SrO})_2$ faults, allowing the rest of the dielectric material to remain stoichiometric. In this work we use MBE to grow RP phases containing $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$, specifically $(\text{SrTiO}_3)_n(\text{BaTiO}_3)_m\text{SrO}$, in hopes of growing thicker films with higher tunability. This is achieved by lowering the epitaxial strain due to BaTiO_3 's smaller mismatch with the DyScO_3 (110) substrate. The first five members of this RP homologous series have been grown on DyScO_3 (110) using MBE and characterized by x-ray diffraction. In-plane measurements of the dielectric constant have been made as a function of temperature and frequency in the gigahertz frequency regime. We use scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) to identify barium and $(\text{SrO})_2$ fault placement, and find high quality films with 1-3 atomic layers of barium interdiffusion.

11:00 AM

(EMA-S12-003-2017) Nanosecond tuning in microwave resonators fabricated on Ruddlesden-Popper thin films

A. M. Hagerstrom^{*1}; X. Lu¹; N. M. Dawley²; H. Nair²; J. Mateu³; J. C. Booth¹; C. J. Long¹; D. G. Schlom²; N. Orloff¹; 1. National Institute of Standards and Technology, USA; 2. Cornell University, USA; 3. Universitat Politècnica de Catalunya, Spain

Consumer demand for higher data rates and lower latencies is pushing the telecommunications industry to develop components that work at higher operating frequencies with improved spectral efficiency. Tunable dielectric materials are the core building blocks of numerous signal-processing technologies that can be used to address these problems. Unfortunately, many of the most widely used tunable dielectrics have high dielectric loss at frequencies above 10 GHz. The only notable exception is $(\text{SrTiO}_3)_n\text{SrO}$ Ruddlesden-Popper (RP) superlattices that have high in-plane tunability, and low dielectric loss at room temperature (loss tangent ~ 0.005) up to at least 125 GHz. Here, we present the first realization of resonant structures, a ubiquitous building block of filters, phase shifters, and multiplexers, utilizing RP thin films. We demonstrate tunability by up to 20% at 200 K and 2.5% at room temperature in these devices, and that this tuning occurs on nanosecond timescales. Our experimental observations are supported by analytical circuit models and finite element simulations.

11:15 AM

(EMA-S12-004-2017) Flip-chip methods for materials characterization from 10 kHz to 110 GHz (Invited)

C. J. Long^{*1}; N. Orloff¹; A. Sahu²; C. Little⁴; I. Hanemann³; A. M. Hagerstrom¹; X. Lu¹; R. Chamberlin¹; V. Devabhaktuni²; T. Wallis⁵; J. C. Booth¹; 1. NIST, USA; 2. University of Toledo, USA; 3. University of Colorado, USA; 4. University of Colorado, USA; 5. NIST, USA

Predicting the performance of fifth-generation (5G) wireless communications devices requires knowledge of a huge range of materials. This includes both the materials that make up a wireless device – for example, metals, semiconductors, polymers, and thin-film dielectrics – and it also includes the materials that wireless signals interact with – for example, concrete, wood, and water. In this talk, I review our efforts to apply flip-chip techniques to characterize the permittivity and permeability of a variety of materials. In our approach, the material under test is placed on top of a set of pre-fabricated and well-characterized coplanar waveguides. Information about the material's properties is then extracted from measurements of the impedance and propagation constant of the waveguides. This approach is non-destructive, quantitative, and yields materials properties across a continuous frequency band from approximately 10 kHz to 110 GHz. The resulting data serves two purposes: it provides feedback to materials designers and it enables more accurate device simulations. In turn, this enables more rapid development of new materials and reduces the number of design iterations required to obtain optimized mm-wave devices.

11:45 AM

(EMA-S12-005-2017) Chemistry, Growth kinetics and Epitaxial Stabilization of Sn^{2+} in Sn-doped SrTiO_3 using $(\text{CH}_3)_6\text{Sn}_2$ precursor (Invited)

T. Wang²; K. C. Pitike¹; Y. Yuan³; S. Nakhmanson¹; V. Gopalan³; B. Jalan^{*2}; 1. University of Connecticut, USA; 2. University of Minnesota, USA; 3. Pennsylvania State University, USA

PbTiO_3 -based ferroelectrics have impressive electroactive properties, originating from the Pb^{2+} $6s^2$ e- lone pair, which cause large elastic distortion & electric polarization due to cooperative Jahn-Teller effect. Recently, tin-based perovskite with Sn^{2+} with $6s^2$ lone-pair, has been identified as a thermally stable, environmentally friendly substitute for PbTiO_3 -based ferroelectrics. However experimental attempts to stabilize Sn^{2+} on the A-site of ATiO_3 have so far failed. We present on the growth of atomically smooth, epitaxial Sn-alloyed SrTiO_3 films on SrTiO_3 (001) using a hybrid molecular beam epitaxy approach. With increasing Sn concentration, the out-of-plane lattice parameter first increases in accordance with the Vegard's law and then decreases for $\text{Sn} > 20$ at% due to the incorporation of Sn^{2+} at the A-site, which is in agreement with density functional theory calculations. A novel yet simple approach using the high-resolution X-ray photoelectron spectroscopy is devised to identify the Sn-site occupation in the lattice of SrTiO_3 . A relaxor-like local ferroelectric distortion with monoclinic symmetry, induced by A-site Sn^{2+} was observed in 21at% Sn-doped SrTiO_3 using optical second harmonic generation measurements. The role of growth kinetics on the solubility of Sn in SrTiO_3 , phase transitions and ferroelectric behavior as a function of Sn will be presented.

12:15 PM

(EMA-S12-006-2017) Combinatorial Methods for Rapid 5G Materials Discovery Demonstrated in $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$

E. Marks^{*1}; N. Orloff²; Y. Liang¹; X. Zhang¹; A. M. Hagerstrom²; X. Lu²; C. J. Long²; J. C. Booth²; I. Takeuchi¹; 1. University of Maryland, USA; 2. National Institute of Standards and Technology, USA

In the simultaneous push to implement a 5G telecommunications network infrastructure and miniaturize the devices operating on such networks, renewed focus has been placed on discovery and understanding of dielectric ceramics exhibiting low loss, high relative permittivity, thermal stability, and even tunability. Here, we have

explored the applicability of combinatorial experimental methods to the search for 5G materials by exploring a well-known system, $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$. Pulsed-laser deposition (PLD) was used to deposit compositionally graded samples with compositions ranging from pure BaTiO_3 to pure SrTiO_3 with a roughly linear compositional gradient. A novel application of established high-frequency dielectric characterization techniques was developed, allowing for the determination of key electronic properties for a range of $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$ compounds. This ability to cofabricate and characterize a compositional library of mm-wave device relevant dielectric ceramics on a single chip may be applied to a wide variety of candidate materials and presents a new opportunity to more rapidly address the needs of the 5G challenge.

S13: Mesoscale Phenomena in Ceramic Materials, Nano- and Microstructures

Synthesis, Characterization and Processing

Room: Coral A

Session Chairs: Serge Nakhmanson, University of Connecticut;
Edward Gorzkowski, Naval Research Lab

10:00 AM

(EMA-S13-001-2017) Caloric responses using ferroelectrics (Invited)

B. Dkhil^{*1}; 1. CentraleSupélec-CNRS, France

Here, we show how to enhance electrocaloric effects using various strategies: multiphase points composition, use of dual-stimuli i.e. stress and electric fields in ferroelectrics to generate multicaloric effects, explore other dual-stimuli by taking advantage of multicaloric effects to switch off the detrimental magnetic losses using an electric field in multiferroic heterostructure, use negative electrocaloric effect revealed in antiferroelectrics as a supplemental tool for designing enhanced caloric responses. B.D. acknowledge Fonds National de la Recherche (FNR) du Luxembourg through the InterMobility project 16/1159210 "MULTICALOR"

10:30 AM

(EMA-S13-002-2017) Complex Domain and Domain Wall Behaviour in Ferroelectrics (Invited)

M. Gregg^{*1}; 1. Queens University Belfast, United Kingdom

Two interesting aspects of domain and domain wall behaviour in ferroelectrics will be discussed: the first concerns the thermodynamic origins of the mesoscale stunningly regular square-net birefringence patterns (or "Forsbergh" patterns) that have been seen to form in certain flux-grown BaTiO_3 single crystals. We have reexamined specific crystals grown by Bell Labs in the 1940's (for Helen Megaw) which show beautiful examples of Forsbergh patterns; however, we see no direct evidence for the intricate tessellating arrangements of domain packets put forward by Forsbergh in his original work [1]. We propose a more mundane explanation for the phenomenon, where complex square-net birefringence arises simply from orthogonally oriented ferroelastic stripe domains overlaying one another. The second topic for discussion concerns conductivity at "charged" domain walls in ferroelectrics. We have recently seen that atomic force microscopy can detect the Hall Effect in these conducting walls. In ytterbium manganite crystals, we have confirmed p-type conduction, but we have also obtained an upper estimate of $\sim 1 \times 10^{16} \text{cm}^{-3}$ for the mobile carrier density in the wall, which is around four orders of magnitude below that required for complete screening of the polar discontinuity. The associated carrier mobility was found to be $\sim 50 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ - an order of magnitude below p-type silicon, but sufficiently high to preclude small polarons.

11:00 AM

(EMA-S13-003-2017) Mesoscopic domain manipulation in ferroelectric/dielectric superlattices (Invited)

J. Park²; Y. Ahn²; A. Pateras²; Q. Zhang³; M. Holt³; J. Mangeri¹; O. Heinonen³; M. Yusuf⁴; M. Dawber⁴; S. Nakhmanson¹; P. G. Evans^{*2}; 1. University of Connecticut, USA; 2. University of Wisconsin, USA; 3. Argonne National Lab, USA; 4. Stony Brook University, USA

Understanding and controlling the spontaneous nanodomain pattern of ferroelectric materials presents both the opportunity to create functionality in nanoscale devices and a series of fundamental challenges. The remnant polarization of ferroelectric/dielectric thin film superlattices exhibit a spontaneous formation of nanodomain patterns with characteristic periodicities at length scales below 10 nm. In as-grown superlattices consisting of many superlattice repeat units, the spatial patterns of domains initially exhibit a short coherence length and a high-degree of disorder in their two-dimensional pattern within the plane of the thin film. A series of experiments illustrate that external perturbations can provide mechanisms to control of the pattern. X-ray diffuse scattering studies of sub-micron lithographic features within the superlattices show that edges induce the alignment of domains. A comparison with finite element calculations including the ferroelectric degree of freedom shows that the aligned domain patterns minimize the free energy through a coupling of the mechanical compliance of the structure with the ferroelectric distortion.

11:30 AM

(EMA-S13-004-2017) Nano to Micro Size Effects in the Mechanical Behavior of Ceramics (Invited)

J. A. Wollmershauser^{*1}; B. N. Feigelson²; H. Ryou³; J. W. Drazin³; E. Gorzkowski¹; K. J. Wahl¹; 1. U.S. Naval Research Laboratory, USA; 2. U.S. Naval Research Laboratory, USA; 3. American Society for Engineering Education, USA; 4. U.S. Naval Research Laboratory, USA

The role of size effects on the exhibited mechanical behavior of ceramics has been a hotly debated topic in the scientific literature. Generally, smaller structures demonstrate improved strength and hardness with structures smaller than 100nm displaying significant increases. However, the source of the increase is often argued to arise from two potential structural sources: geometric size of the mechanical test or the size of the crystallites comprising the ceramic. The former is commonly called an indentation or sample size effect while the latter is referred to as a grain size effect (i.e., Hall-Petch relationship). Recent novel developments in processing of bulk nanostructured ceramics have opened the door to create fully dense volumetric ceramics with grain sizes much smaller than 100nm. With these new materials in hand and advances in indentation instrumentation, the fundamental physical behavior across all grain size ($\sim 10\text{nm}$ to single crystal) and indentation length scales (nano to micro) can be explored. For example, the distinct contributions from each size effect can be effectively determined at specific length scales ranging from 10s of nm to 10s of microns. Such an understanding of the mechanical response of dense bulk ceramics is paramount before seriously considering their use in DOD applications.

S14: Multifunctional Nanocomposites

Multifunctional Nanocomposites: Functionality by Design I

Room: Caribbean C

Session Chair: Aiping Chen, Los Alamos National Lab

10:00 AM

(EMA-S14-001-2017) Colossal ionic conductivity discovered in interfacial quantum oxide nanostructures (Invited)

H. Lee^{*1}; 1. Oak Ridge National Laboratory, USA

Discovery of high performance ionic conductors is an important stepping-stone to next generation energy and environmental technologies. Over the last decade, one-dimensional nanostructures have shown the feasibility as a new type of ionic electrolytes. However, controlled growth of high quality nanocrystals is challenging especially for ionic oxide materials. In this work, using pulsed laser epitaxy, we report significantly increased oxygen ion conduction in highly porous micron-thick nanobrush superlattices composed of unitcellthin binary oxides, including CeO_2 , which are one dimensional, vertically aligned, and single crystalline. Through electrochemical impedance spectroscopy, we found that the ionic conductivity of the oxide nanosuperlattices was enhanced by up to two orders of magnitude as compared to yttria-stabilized zirconia. The ionic conductivity is also exceedingly large compared to doped ceria. Thus, this presentation will focus on unveiling the underlying mechanism on the growth of such unique crystalline nanobrushes and the origin of the improved ionic conductivity. Our finding provides deeper insight into improving oxygen ion conduction in a form of quantum heterostructures and a means to develop high performance oxygen ion conductors. * This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:30 AM

(EMA-S14-002-2017) Novel Vertically Aligned Nanocomposite (VAN) Designs: Oxide-oxide systems and beyond (Invited)

H. Wang^{*2}; L. Li³; W. Zhang⁵; J. Huang¹; J. Jian⁴; M. Fan⁴; Q. Su⁶; X. Sun¹; X. Wang¹; J. MacManus-Driscoll¹; Q. Jia⁸; 1. Purdue University, USA; 2. Purdue University, USA; 3. Texas A&M University, USA; 4. Texas A&M University, USA; 5. Texas A&M University, USA; 6. Texas A&M University, USA; 7. University of Cambridge, United Kingdom; 8. SUNY Buffalo, USA

Vertically aligned nanocomposites (VAN) in epitaxial form provide a novel platform for enabling strain coupling of two phases through film thickness, creating charge carrier barriers for flux pinning in superconductors and electrical transport paths in magnetoresistance materials, providing fast ionic transport paths for ionic conducting systems, and coupling functionalities of two phases for novel multifunctional materials. This talk reviews examples in all these areas and presents the new findings in VAN designs beyond oxide-oxide systems. These new findings open the VAN field to a new paradigm with enormous opportunities in functional material designs.

11:00 AM

(EMA-S14-003-2017) Emergent Phenomena at Oxide Interfaces: Electronic Reconstruction Induced Ferromagnetism in a Polar Antiferromagnetic Insulator (Invited)

L. W. Martin^{*1}; 1. University of California, Berkeley, USA

Electronic reconstruction and emergent phenomena at the interface between polar and non-polar oxides has been the focus of considerable research. Beyond $\text{LaAlO}_3/\text{SrTiO}_3$, work on $\text{LaMnO}_3/\text{SrTiO}_3$ has proposed that charge transfer occurs within the insulating, polar LaMnO_3 as a result of a potential build-up which produces electron doping near the interface and ferromagnetism. Direct evidence for this electronic reconstruction and the nature of magnetism, however, has not been reported. Here we provide direct evidence

of electronic reconstruction and ferromagnetism within the polar, antiferromagnetic insulator LaMO_3 grown on nonpolar SrTiO_3 . X-ray absorption spectroscopy reveals electronic reconstruction in the LaMnO_3 (reduction of Mn near the interface) even in 2 UC thick films, but no valence change in the SrTiO_3 . This reconstruction induces X-ray magnetic circular dichroism (XMCD) at the Mn $L_{2,3}$ -edges consistent with ferromagnetism. Theory shows that the electric potential build-up in the LaMO_3 is $0.177 \text{ V}/\text{\AA}$, resulting in a critical thickness for electronic reconstruction of only 2 UC. Using a chemical route we dope the material thereby strengthening the magnitude of the ferromagnetic order such that XMCD signals can be observed in films down on only 3 UC.

11:30 AM

(EMA-S14-004-2017) Interfacial Tuning of Leakage Current and Hysteresis Behavior in Vertically Aligned Nanocomposite Thin Films

E. Enriquez^{*1}; A. Chen¹; P. C. Dowden¹; Z. Harrell²; L. Li³; D. Xue¹; N. Koskela¹; J. Roback¹; J. MacManus-Driscoll¹; H. Wang³; C. Chen²; Q. Jia⁵; 1. Los Alamos National Lab, USA; 2. University of Texas at San Antonio, USA; 3. Texas A&M University, USA; 4. University of Cambridge, United Kingdom; 5. University at Buffalo, State University of New York, USA

The interface between two materials in a nanocomposite thin film represents a region of tremendous importance for the resulting modifications to a material's intrinsic structural, physical, electrical and magnetic transport properties. The presence of oxygen vacancies at the interface is critical to controlling interfacial behavior and material interaction in complex oxide nanocomposites. In this work, we explore the effect of oxygen vacancy concentration on the conduction behavior of epitaxial vertically aligned nanocomposite thin films via various annealing conditions. It was found that structure and conduction behavior depends greatly on the oxygen content. We employ models that indicate that hysteretic conduction can be reliably modulated by concentration of oxygen vacancies at the vertical heterointerface. Our results emphasize the critical role of oxygen vacancy behavior at the interface in vertically aligned nanocomposite thin films, and further illustrate the potential to tune functionalities via control of synthesis and processing conditions.

11:45 AM

(EMA-S14-005-2017) Sub-Surface Grain and Domain Boundary Imaging for Functional Thin Films

B. D. Huey^{*1}; J. Steffes¹; T. Green¹; L. Ye¹; 1. University of Connecticut, USA

Multifunctional nanocomposites typically leverage the advantages and distinct functionalities of their discrete phases, as well as further enhancements due to cross-coupling between the composite components. Local property measurements, however, are limited to either bulk studies or surface investigations as with atomic force microscopy. In this work, cross-sectional property maps into the depth of functional thin films are prepared. The sub-surface angles of domain walls, and grain boundary microstructure, are thus uniquely revealed, concomitant with their effects on local functional properties. This approach thereby provides numerous opportunities to contribute to multifunctional nanocomposite research.

12:00 PM

(EMA-S14-006-2017) Uncovering the atomic scale origins of functionality in oxide nano composites via scanning transmission electron microscopy (Invited)

J. M. LeBeau^{*1}; E. D. Grimley²; T. Schenk³; U. Schroeder⁴; X. Sang¹; 1. North Carolina State University, USA; 2. North Carolina State University, USA; 3. Namlab, Germany; 4. Namlab, Germany

The functionality of nanocomposite oxide thin films is intimately linked to atomic structure. To reveal the small scale displacements that occur in these structures, scanning transmission electron microscopy (STEM) has provided critical insights, for example at interfaces, defects, or dopants. In this talk, I will highlight our work

using state-of-the-art STEM to characterize the structure and chemistry of oxide thin films. Multiple case studies will be presented to demonstrate the power of new STEM techniques, such as revolving STEM and position averaged CBED, to characterize thin films. For example, I will show how RevSTEM images can be used to accurately determine crystallographic parameters in real-space, and to determine the structural origins of polarization in ferroelectric HfO₂ thin films. We also identify the presence of thin, non-uniform tetragonal hafnia layers at the electrode/ferroelectric interfaces with the bulk of the grains being monoclinic or orthorhombic. The evolution of these phases with field-cycling are then correlated with changes in the ferroelectric response. Overall, this talk will emphasize a new world of atomic scale exploration that was previously just beyond reach.

S15: Superconducting Materials and Applications

New Superconducting Materials and Phenomena I

Room: Pacific

Session Chairs: Xingjiang Zhou, Chinese Academy of Sciences;

Jin-Feng Jia, Shanghai Jiao Tong University

10:00 AM

(EMA-S15-001-2017) Tuning phase transitions of FeSe thin flakes by field effect transistor with solid ion conductor as gate dielectric (Invited)

X. Chen^{*1}; 1. University of Science and Technology of China, China

So far, there are only two types of field effect transistor (FET) devices, metal-insulator-semiconductor (MIS) FET and electric double layer (EDL) FET, which can be widely used to continuously tune carrier density. However, there are inherent drawbacks. The MIS-FET can only sustain very limited carrier density, while the overlay of liquid electrolyte in EDL-FET obstructs its applications in modern electronic technology and prevents heavily-doped electronic states from being characterized by many physical measurements. In this talk, I will report on a novel FET device with solid ion conductor (SIC) as a gate dielectric to overcome the inherent drawbacks of both MIS- and EDL-FET devices. Using this FET device, we can tune the carrier density of FeSe by driving lithium ions in and out of the FeSe thin flakes, and consequently control the material properties and its phase transitions. A dome-shaped superconducting phase diagram was mapped out with increasing Li content, with $T_c \sim 46.6$ K for the optimal doping, and an insulating phase was reached at the extremely overdoped regime. Our study suggests that, using solid ion conductor as a gate dielectric, the SIC-FET device can achieve much higher carrier doping in the bulk, and suit many surface sensitive experimental probes, and can stabilize novel structural phases that are inaccessible in ordinary conditions.

10:30 AM

(EMA-S15-002-2017) Strategy and progress on exploration of new superconductors (Invited)

G. Cao^{*1}; 1. Zhejiang University, China

Exploration of new superconductors is at the forefront of superconductivity research, which is very challenging as well. In this talk I will share with the audience on the general strategies for exploring new superconductors. With these strategies, we were able to make progress along this direction in recent years. We hope such strategies could be helpful to make continuous findings in the future.

11:00 AM

(EMA-S15-003-2017) Single crystal growth and basic thermodynamic and transport properties of 1144 superconducting compounds (Invited)

S. L. Bud'ko^{*1}; 1. Ames Laboratory / Iowa State University, USA

An overview of first successful single crystal growth and anisotropic physical properties of CaKFe₄As₄ will be given. Basic superconducting parameters are inferred and discussed. There is no indication of any phase transition, other than superconductivity with $T_c = 35.0 \pm 0.2$ K, taking place in this compound for $1.8 \text{ K} < T < 300 \text{ K}$. All of the data, including pressure dependence of T_c indicate that stoichiometric CaKFe₄As₄ is intrinsically close to what is referred to as "optimal-doped" on a generalized, Fe-based superconductor, phase diagram.

11:30 AM

(EMA-S15-004-2017) Searching for Superconductors in Complex Mixtures: Solid-state Synthesis, Structural Analysis, and Physicochemical Characterization (Invited)

J. Brant^{*1}; D. C. Vier²; T. Bullard¹; T. J. Haugan¹; 1. Air Force Research Lab, USA; 2. University of California, San Diego, USA

Our search for new high-temperature superconductors is guided by common structural features and compositions that are shared by superconductors in a variety of material families. Since superconductivity is often ascribed to specific layers within a crystal structure, new materials with layered structures are targeted using conventional high-temperature solid-state synthesis. Here, Magnetic Field-Modulated Microwave Spectroscopy (MFMMS), which can be used to selectively detect superconducting transitions with high sensitivity and selectivity, is used to search for signatures of superconductivity in polycrystalline powders. Magnetic Field-Modulated Microwave spectra of RE-M-O (RE = rare earth; M = transition metal) samples exhibited responses that are akin to those from superconductors, such as YBCO. The structures and phase compositions were analyzed via X-ray powder diffraction (XRPD). In some cases, high resolution synchrotron XRPD data was used to assess low-weight fraction phases in samples that gave rise to peak-like responses in MFMMS data. Rietveld refinements using high-resolution XRPD data allowed the phases in complex mixtures to be identified and quantified. Zero-field cooled (ZFC) and field-cooled (FC) vibrating sample magnetometry (VSM) was used to evaluate magnetic properties.

12:00 PM

(EMA-S15-005-2017) Interface superconductivity in undoped CaFe₂As₂ and rare earth doped CaFe₂As₂

L. Deng^{*1}; K. Zhao¹; B. Lv²; Z. Wu¹; S. Huyan¹; Y. Xue¹; C. Chu¹; 1. Texas Center for Superconductivity at the University of Houston, USA; 2. University of Texas at Dallas, USA

Superconductivity has been reversibly induced/suppressed in undoped CaFe₂As₂ (Ca122) single crystals through proper thermal treatments, with T_c at ~ 25 K at ambient pressure and up to 30 K at 1.7 GPa. We found that Ca122 can be stabilized in two distinct tetragonal phases (T) at room temperature and ambient pressure: PI with a non-magnetic collapsed tetragonal (cT) phase at low temperature and PII with an antiferromagnetic orthorhombic phase (O) at low temperature. Detailed X-ray diffraction profile analyses further reveal mesoscopically stacked layers of the PI and the PII phases. The results provide the most direct evidence to date for interface-enhanced superconductivity in undoped Ca122, consistent with the recent theoretical prediction. To explore the origin of the unusual non-bulk superconductivity with a T_c up to 49 K reported in the rare earth-doped Ca122 [(Ca,R)122], the chemical composition, magnetization, specific heat, resistivity, and annealing effect are systematically investigated on nominal (Ca,R)122 single crystals with different x and R = La, Ce, Pr, and Nd. Our observations provide evidence for the crucial role of defects in the occurrence of

the unusually high $T_c \sim 49$ K in this system and are consistent with the interface-enhanced superconductivity recently proposed.

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Material Design, Fabrication and Applications II

Room: Indian

Session Chairs: Andrew Bell, University of Leeds; Fei Li, Xi'an Jiaotong University

2:00 PM

(EMA-S1-009-2017) Relaxor-based Ferroelectrics: Ultrahigh Piezoelectric Activity from Polar Nanoregions (Invited)

F. Li^{*2}; S. Zhang¹; L. Chen³; T. Shrout³; 1. University of Wollongong, Australia; 2. Xi'an Jiaotong University, China; 3. Pennsylvania State University, USA

A breakthrough in ferroelectric materials is the discovery of ultrahigh piezoelectric responses of relaxor-ferroelectric single crystals. A key signature of relaxor-ferroelectrics is the existence of polar nanoregions (PNRs), a nano-scale inhomogeneity. Despite two decades of active studies, the contribution of PNRs to the piezoelectric properties has yet to be established. Here, we quantitatively characterize the contribution of PNRs to the dielectric/piezoelectric response of relaxor-ferroelectric crystals using a combination of cryogenic experiments and phase-field simulations. We find that the contribution of PNRs accounts for 50-80% of the room-temperature dielectric and piezoelectric responses. We propose a new mesoscale mechanism to reveal the origin of the high piezoelectric properties in relaxor-ferroelectric crystals, where the "collinear" PNRs act as "seeds" for the polarization rotation. This mechanism emphasizes the critical role of the local structure and order on the macroscopic properties of ferroelectric materials, which is expected to guide the exploration of next generation high performance ferroic materials.

2:30 PM

(EMA-S1-010-2017) Mechanisms for the Low Temperature Dielectric Relaxation in Lead Titanate-Relaxor Single Crystals (Invited)

A. J. Bell^{*1}; 1. University of Leeds, United Kingdom

The mechanism of the low temperature dielectric relaxation and reduction in piezoelectric charge coefficient is crucial to understanding large piezoelectric coupling in $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - PbTiO_3 (PMN-PT) type single crystals at room temperature. Over the last decade, the room temperature mechanism has generally been understood in terms of polarization rotation between rhombohedral and tetragonal variants through a shallow free-energy landscape, which does not explicitly involve a temperature activated mechanism that would lead to a relaxation response. On the other hand, a similar relaxation in PZT ceramics can be attributed to the freezing of domain walls, which does imply a temperature activated mechanism. Recently Li et al have proposed a mechanism involving the freezing of polar nanoregions, in which the frozen regions exhibit a polar axis rotated from that of the matrix. This paper considers the microscopic mechanism of polarization rotation. It shows how the short coherence length of polarization, evident in the higher temperature paraelectric-(relaxor)-ferroelectric transition, can impart thermal activation to the polarization rotation mechanism, through domains or PNRs. The model is supported by a statistical mechanics treatment of the Landau-Devonshire free energies of PMN and PZT. The resulting low temperature relaxation is consistent with that seen experimentally.

3:00 PM

(EMA-S1-011-2017) Comparing "Simple" Perovskites: NSMM Versus Goldschmidt's Tolerance Formalism

S. C. Tidrow^{*1}; 1. Alfred University, USA

Experimental data of roughly one-hundred "simple" Perovskites are compared with the Goldschmidt's (conventional) tolerance formalism, which is celebrating 90 years, as well as compared with an evolving new "simple" material model (NSMM), which uses spreadsheet calculations. NSMM is shown to significantly outperform Goldschmidt's tolerance formalism at room temperature for determination of lattice structure, lattice parameter, and volume. In addition to extending such improved performance over large temperature ranges, NSMM is importantly able to address temperature dependent permittivity as well as locate the temperature range of polarization induced structural phase transitions. Also importantly, NSMM has been used to show that the Clausius-Mossotti equation (permittivity) or equivalently the Lorentz-Lorenz equation (index of refraction) incorporates the Curie Law and Curie-Weiss Law, with the latter two being correlation relations not laws, through use of genome-like ion properties, temperature dependent radii and polarizability, which define the temperature dependent lattice volume, the Curie temperature (T_c) and the Curie constant (C).

3:15 PM

(EMA-S1-012-2017) Enhanced Q, Dielectric Constant 80 Microwave Dielectric Materials for LTE Applications

M. D. Hill^{*1}; 1. Trans-Tech Inc., USA

Modern low frequency LTE applications require enhanced Q, temperature stable materials with dielectric constants between 70 and 90. Although the $\text{Ba}_{6-3x}\text{Ln}_{8+2x}\text{Ti}_{18}\text{O}_{54}$ system has been well studied and has the highest dielectric constant values of any temperature compensated system, Q values are currently insufficient for modern LTE applications. However, with substitutions of aluminum and/or germanium for titanium on the octahedral site, polycrystalline ceramic materials with Qf products in the 10000 – 11000 range at 1 GHz may be obtained. The addition of tantalum or niobium oxide will dramatically increase the dielectric constant allowing for temperature stable materials with dielectric constants close to 80.

Characterization of Materials: Crystal Structure and Properties I

Room: Indian

Session Chair: Jacob Jones, North Carolina State University

4:00 PM

(EMA-S1-013-2017) Capturing Quantitative Static and Dynamic Local Structure with Scanning Transmission Electron Microscopy (Invited)

J. M. LeBeau^{*1}; 1. North Carolina State University, USA

Electron microscopy has been revolutionized by the aberration corrector, which dramatically improves spatial resolution into the sub-ångström regime. This has unlocked previously inaccessible information about material structure. While these recent advances have proven essential to the atomic scale characterization of materials, accuracy and precision for scanning transmission electron microscopy (STEM) was significantly hampered by the presence of sample drift and scan distortion. This limitation had obscured the capabilities to characterize minute changes to the atomic structure that can ultimately define material properties. In this talk, I will introduce revolving scanning transmission electron microscopy (RevSTEM). The method uses a series of fast-acquisition STEM images, but with the scan coordinates rotated between successive frames. Multiple case studies will be presented to highlight the power of this new technique to characterize materials. For example, I will show how picometer precise measurements enable the

capability to directly observe static atomic displacements within a complex oxide solid solution exhibiting differences in local bonding. Moving beyond static experiments, I will also highlight our recent work on imaging (110) SrTiO₃ surface dynamics via in-situ STEM at temperatures up to 900 C.

4:30 PM

(EMA-S1-014-2017) In situ X-ray investigation of Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ polycrystalline ceramics in an external electric field

D. Hou^{*1}; T. Usher²; M. Vrabelj³; L. Fulanovic³; H. Ursic³; B. Malic³; I. Levin⁴; J. L. Jones¹; 1. North Carolina State University, USA; 2. Oak Ridge National Laboratory, USA; 3. Jozef Stefan Institute, Slovenia; 4. National Institute of Standards and Technology, USA

Relaxor-ferroelectrics in (1-x)Pb(Mg_{1/3}Nb_{2/3})O₃-xPbTiO₃ (PMN-PT) can exhibit a high dielectric permittivity, polarization, and piezoelectricity. Recently, the electrocaloric effect has been reported in PMN-PT polycrystalline ceramics, showing potential applications in a new generation of cooling devices. The electrocaloric effect in PMN-PT may be related to the change in polarization when subjected to an electric field. However, to our best knowledge, the mechanism of this polarization change is still unclear. Here, the electric-field-dependent structure of PMN-0.3PT ceramics was studied using in situ X-ray diffraction and total scattering. In situ diffraction patterns indicate a field-induced and long-range series of phase transitions. Rietveld refinements of the diffraction patterns suggest a Cm (monoclinic M_A) to Pm (monoclinic M_C) to P4mm (tetragonal) transition with increasing field. This transition sequence can be explained by the polarization rotation mechanism, which has only been experimentally shown in PMN-PT single crystals, but not yet in polycrystalline ceramics. In situ total scattering studies suggest a [001] tetragonal distortion at local scale, and the distortion is enhanced systematically under fields. In summary, our results show unique structural insight to the polarization rotation mechanism in polycrystalline relaxor-ferroelectrics

4:45 PM

(EMA-S1-015-2017) Evidence of Structural Changes that Drive Wake-up and Fatigue in Ferroelectric Hafnia

E. D. Grimley^{*1}; T. Schenk²; X. Sang³; M. Pešić²; U. Schroeder²; T. Mikolajick⁴; J. M. LeBeau¹; 1. North Carolina State University, USA; 2. NaMLab gGmbH, Germany; 3. Oak Ridge National Laboratory, USA; 4. NaMLab gGmbH / TU Dresden, Germany

As research on ferroelectric thin film HfO₂ continues gaining momentum, considerable efforts are now seeking to minimize wake-up and fatigue induced changes in the ferroelectric hysteresis, as they prevent its incorporation into stable non-volatile memories. Here, we utilize advanced electron microscopy techniques to correlate field-cycling induced electrical changes to structural changes. We identify the presence of thin, non-uniform tetragonal hafnia layers at the electrode/ferroelectric interfaces, in spite of the phase of the bulk grains always being monoclinic or orthorhombic. These interfacial layers are proposed to form during growth as the electrodes are oxidized, which leaves behind oxygen vacancies. These charged defects stabilize thin tetragonal layers and produce internal bias fields in pristine devices. Field-cycling reduces the presence of these layers, eliminating bias fields. Further, our results suggest a monoclinic to orthorhombic phase change in the bulk grains, which is proposed as one reason for the increased remanent polarization of the woken-up films. Lack of obvious structural changes with further cycling until fatigue, in conjunction with static leakage current and other electrical measurements, suggests defect generation in the bulk. These results are augmented by impedance spectroscopy and electrical modeling, which will be discussed.

5:00 PM

(EMA-S1-016-2017) X-ray Study of Amorphous to Crystalline Transition of In-M-O (M: Sn, Zn, Ga) Thin Films

L. Zeng^{*1}; M. M. Moghadam²; D. B. Buchholz²; R. Chang²; P. W. Voorhees²; T. J. Marks³; M. J. Bedzyk²; 1. Northwestern University, USA; 2. Northwestern University, USA; 3. Northwestern University, USA

Amorphous metal oxides (AMOs) are the key channel layer materials of thin film transistors (TFTs) for future electrical applications due to the unique properties of combination of optical transparency, high mobility, low deposition temperature, and low-cost. So far, excessive attention has been paid to tune and optimize electrical properties while little research has been done on the thermal properties of AMOs materials. Herein, an in situ experiment by employing synchrotron X-ray technique has been carried out to characterize the isochronal crystallization process of AMO thin films deposited by pulsed-laser deposition (PLD). A series of (In_{1-x}M_x)₂O₃ thin films were deposited as a function of doping concentration x (x=5%, 10%, 20% and 30%) for M=Sn, Zn and Ga respectively. In situ grazing incident wide-angle X-ray scattering (GIWAXS) technique coupled with an area detector was used to monitor and record the amorphous to crystalline transition of (In_{1-x}M_x)₂O₃ thin films under isochronal annealing condition (constant ramping rate). Time-sequenced 2D diffraction images were collected and subsequently analyzed to subtract the degree of crystallinity evolution for each element. The 2D diffraction patterns of the crystalline thin films after the annealing process can also provide information such as lattice constant variation, phase separation, crystallites orientation, and surface morphology.

5:15 PM

(EMA-S1-017-2017) Direct observation of local chemistry and local cation displacements in the relaxor ferroelectric Pb(Mg_{1/3}Nb_{2/3})O₃ (PMN)

M. J. Cabral^{*1}; S. Zhang²; E. C. Dickey¹; J. M. LeBeau¹; 1. North Carolina State University, USA; 2. University of Wollongong, Australia

Picometer-scale lattice distortions play an important role on the macroscopic properties of relaxor ferroelectric materials. Due to competition between composition/charge ordering in these materials, there is a formation of "polar nanoregions" (PNRs) and chemically ordered regions (CORs) where local chemical fluctuations on the B-site give rise to inhomogeneities in local strain and polarization on the nanometer scale. Direct real-space visualization of these distortions and local chemical composition can provide important insight to the formation and relationship of both PNRs and CORs. Using aberration-corrected STEM combined with advanced imaging methods we directly observe atom column specific, picometer scale displacements in the relaxor ferroelectric lead magnesium niobate (PMN). In this talk, we provide a study of local polarization and its relation with local chemistry in PMN. Additionally, we show the scale of chemical ordering using atomic resolution EDS and STEM image quantification. Atomic resolution, in-situ STEM studies provide insight into the local structure and chemical ordering of PMN above and below the Burns temperature. Combining experiment with STEM image simulation, we are able to provide direct correlations between compositional disorder and local polarization in these complex relaxor ferroelectric materials.

S2: Advanced Processing for Electronic and Electrochemical Systems: Crystals, Films and Devices

Refined Synthesis Routes to Advance and Enable Properties II

Room: Coral B

Session Chair: Jon-Paul Maria, North Carolina State University

2:00 PM

(EMA-S2-008-2017) Doping control in epitaxial CdO thin films by RF and pulsed-DC reactive co-sputtering

K. Kelley^{*1}; J. Maria¹; E. Sachet¹; I. North Carolina State University, USA

In recent years, conductive oxides have been increasingly investigated in the context of plasmonics. While plasmonic materials for UV-VIS and near infrared wavelengths have been found, the mid-infrared range remains a challenge to address. Recent developments show Dy-doped CdO (CdO:Dy) grown via molecular beam epitaxy (MBE) can achieve electron mobilities ($\sim 500 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$) and carrier densities (10^{20} cm^{-3}) that satisfy the criteria for mid-infrared spectrum plasmonics. However, MBEs limited throughput and high cost present a barrier towards larger scale application of this material. Previously, we have shown that CdO:Dy grown via reactive RF co-sputtering is a viable alternative to MBE offering a more accessible route towards ubiquitous IR plasmonic technologies based on CdO. In this work, we identify yttrium as a candidate dopant with a relatively new deposition technique known as RF assisted reactive pulsed DC co-sputtering. We show that epitaxial films grown by this method exhibit electrical and optical properties comparable to MBE grown materials. Experiments thus demonstrate co-sputtered CdO:Y on Al_2O_3 with carrier densities of 10^{20} cm^{-3} and mobilities in excess of $400 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. Furthermore, we demonstrate that carrier density can be reproducibly tuned between low 10^{19} cm^{-3} and mid 10^{20} cm^{-3} by controlling the magnetron power and the cathode to substrate distance for the dopant source.

2:15 PM

(EMA-S2-009-2017) Structural Distortions and Composition Trends in Entropy-Stabilized Thin Films

G. N. Kotsonis^{*1}; D. Brenner¹; D. Harris¹; Z. Rak¹; C. M. Rost¹; J. Maria¹; I. North Carolina State University, USA

Entropy stabilized oxides (ESOs) are a novel class of material that feature a conventional oxygen anion sublattice in conjunction with a cation sublattice that is randomly populated by five or more different metal cations. The first published ESO was an equimolar mixture of MgO, CoO, CuO, NiO, and ZnO that converged to a single-phase rocksalt structure above 900°C using traditional bulk ceramic techniques. Notably, the high configurational entropy allows Cu and Zn to exist in a coordination state that is not usually favorable under ambient conditions. Using vapor deposition techniques, the number of ESO formulations can be expanded dramatically. These compositions include cations with a greater deviation of size, mass, or valence preference than the original ESO composition. In this presentation we demonstrate how the kinetic energy of incoming adatoms contributes to the TS term, enabling one to freeze in entropically stabilized structures at room temperature. These extreme non-equilibrium phases exhibit pronounced structural distortions that depend upon deposition conditions and the charge state of the "misfit" cations. We focus on the Sc and Cr-containing ESO's and show how deposition temperature can control the tetragonal distortion of epitaxial films on MgO. Finally, we will present X-ray absorption spectroscopy data showing how these distortions are coupled to cation oxidation states.

2:30 PM

(EMA-S2-010-2017) Thermal Properties of Entropy-Stabilized Oxides

J. Braun³; A. Giri⁴; C. M. Rost¹; D. Brenner⁵; J. Maria⁵; P. Hopkins^{*2};

1. University of Virginia, USA; 2. University of Virginia, USA; 3. University of Virginia, USA; 4. University of Virginia, USA; 5. North Carolina State University, USA

High entropy alloys (HEAs) were created by incorporating five or more elemental species of metals into a single lattice with random occupancy. This concept inspired the creation of five-component oxides; by populating a single sublattice with many distinct cations, oxides that contain high configurational entropy and are entropy-stabilized have been demonstrated. Fabricated in bulk form via bulk ceramics processing, this entropy-stabilized oxide system is an equimolar mixture of MgO, CoO, NiO, CuO and ZnO, each component chosen to provide diversity in structures, coordination and cationic radii. A thin-film layer of this entropy-stabilized oxide system was grown via sputter deposition on an MgO substrate. These novel materials present a unique opportunity to study the thermal properties and heat carrier characteristics of a new material system. Here, we report on the thermal conductivity and heat capacity of a 300 nm entropy stabilized oxide system described above. Moreover, we use this system to determine a thermal conductivity model that can be applied to entropy-stabilized oxides having different constituents. In so doing, we reveal the nature of phonon transport and phonon scattering within this material system.

2:45 PM

(EMA-S2-011-2017) Structure-Process-Property Relationships in HfN thin films on sapphire

K. Ferri^{*1}; C. M. Rost²; P. Hopkins²; E. D. Grimley¹; J. M. LeBeau¹; J. Maria¹;

1. North Carolina State University, USA; 2. University of Virginia, USA

HfN thin films are generating new interest as substrates for fluoride-based ferroelectric thin films, and for high temperature reflectance thermometry applications. In both cases it is critically important to ensure tight control of resistivity, phase, crystal orientation, and surface topography. In this presentation we will demonstrate how processing parameters including temperature, pressure, and Ar:N_2 ratio influence the crystal structure, topography, phase, and transport properties of reactive sputtered HfN on c-plane sapphire. Substrate temperature and N_2 flow rate were found to have the most significant effect on both film crystallinity and resistivity. The Ar:N_2 ratio has profound impacts on phase evolution. Phase-pure HfN can be grown at a ratio of 35:1, but increasing or decreasing this ratio by as little as 10 % can promote N-rich or N-deficient phases respectively. Increasing substrate temperature from RT to 425°C on sapphire substrates at the optimized gas ratio promotes a transition from mixed orientation to 111 epitaxy. Films prepared in the range of 400°C exhibit resistivity values below $20 \mu\Omega \bullet \text{cm}$ and surface roughness RMS values of 105 nm. Finally, we present preliminary data demonstrating that HfN can be used as a transducer material for TDTR thermometry measurements, particularly at high temperatures.

3:00 PM

(EMA-S2-012-2017) Exploiting kinetics and thermodynamics to grow PbTiO_3 by MBE with continuous codeposition of source elements

E. Smith^{*1}; K. Parrish²; H. Paik¹; J. Schubert⁴; T. Heeg⁵; J. Grazul³;

J. A. Malen²; D. G. Schlom¹; 1. Cornell University, USA; 2. Carnegie Mellon University, USA; 3. Cornell Center for Materials Research, USA; 4. Forschungszentrum Jülich GmbH, Germany; 5. Heeg Vacuum Engineering, Germany

Adsorption-controlled growth, which uses thermodynamics to grow high-quality single-phase materials from non-stoichiometric starting materials, is the standard way of growing compound semiconductors by MBE. In addition, it is used to grow a variety of

superconducting, ferroelectric, and multiferroic materials such as $\text{Bi}_2\text{Sr}_2\text{CuO}_6$, PbTiO_3 , and BiFeO_3 . Because of difficulty in oxidizing Pb, adsorption-controlled growth of PbTiO_3 generally either uses an oxidized Pb precursor (e.g. PbO) or includes “wait” steps or shuttling of the Ti source, slowing down growth times and exposing the growing film to changing growth conditions. We grow PbTiO_3 thin films by MBE utilizing continuous codeposition for the first time. These films are of high crystallographic quality, with rocking curve full-width half maxima as low as 0.011° , equal to that of the substrate and smaller than any other value reported for thin films of PbTiO_3 . We grow PbTiO_3 films on SrTiO_3 (001) substrates with all domains oriented with polarization parallel to the substrate normal; films with thicknesses ranging from 20 nm up to 130 nm are grown with this morphology. We present results that use frequency domain thermoreflectance to characterize the dependence of the cross-plane thermal conductivity on film thickness.

3:45 PM

(EMA-S2-013-2017) Enhanced Electrical Resistivity and Properties via Ion Bombardment of Ferroelectric Thin Films

S. Saremi^{*1}; R. Xu¹; L. Dedon¹; J. Mundy¹; S. Hsu¹; Z. Chen¹; A. Damodaran¹; S. Chapman²; J. T. Evans²; L. W. Martin¹; 1. University of California, Berkeley, USA; 2. Radiant Technologies Inc., USA

Deterministic control of electronic conduction is critical for a range of modern devices. In semiconductors, for example, considerable effort goes into defining where and when the material will be insulating or conducting. In turn, techniques such as ion bombardment, have been developed to tune the electrical conduction by controlled defect formation. In this work, we demonstrate enhanced resistivity and properties in ion-bombarded ferroelectric PbTiO_3 . As-grown, highly-crystalline, stoichiometric PbTiO_3 films suffer from crippling electrical leakage that precludes utilization of the material in a device. In turn, defects induced by in situ knock-on damage during growth or ex situ via ion bombardment are found to systematically reduce electrical leakage currents by 5 orders of magnitude, and improve the ferroelectric device performance. A combination of impedance spectroscopy, temperature-dependent current-voltage, and deep-level transient spectroscopy studies reveal no change in conduction mechanism, but systematic changes in the trap energy from 0.24-0.27 eV in as-grown, pristine films to 0.93-1.01 eV for the ion-bombarded films which corresponds to a complete quenching of shallow trap states. The improved electrical performance is attributed to the formation of knock-on-damage induced defect complexes and clusters which produce deeper trap states and reduce free carrier transport.

4:00 PM

(EMA-S2-014-2017) Semiconductor-to-metal phase transition of VO_2 thin films on soda-lime glass substrates

J. Jian^{*3}; A. Chen¹; W. Zhang⁴; C. Jacob²; H. Wang³; J. Huang³; H. Wang³; 1. Los Alamos National Lab, USA; 2. Texas A&M University, USA; 3. Purdue University, USA; 4. Brookhaven National Laboratory, USA

Vanadium dioxide (VO_2) has drawn great research interests in the past decades owing to its unique semiconductor-to-metal phase transition (SMT) and the corresponding resistance switching properties. In this work, VO_2 thin film was deposited on amorphous glass substrate by pulsed laser deposition. It showed excellent SMT properties with a sharp transition width ($\sim 4.3^\circ\text{C}$) and large transition amplitude (3.2×10^3) compared to the ones on c-cut sapphire and Si (111) substrates. The outstanding SMT properties are correlated with the large grain size and low defects density of the film. Furthermore, by varying the grain sizes of VO_2 films on glass substrates, it showed that the films with larger average grain sizes exhibit better phase transition properties, i.e. higher transition amplitude and sharper transition width. A high resolution TEM study at GB areas revealed the disordered atomic structures along the boundaries and the distorted crystal lattices near the boundaries, which results in the drop of the film SMT properties.

*Denotes Presenter

Advanced Processing for Photoelectrochemistry

Room: Coral B

Session Chair: Kyle Kelley, North Carolina State University

4:15 PM

(EMA-S2-015-2017) High Performance Metal-Insulator-Semiconductor Photosynthesis Cells (Invited)

P. McIntyre^{*1}; 1. Stanford University, USA

Photoelectrolysis is of interest for direct solar-driven production of chemicals and fuels. A persistent challenge in this field is the difficulty of simultaneously achieving high photovoltaic efficiency and chemical stability of semiconductor photoelectrodes during water oxidation. In 2011, Chen et al. demonstrated that atomic layer deposition (ALD) of a thin TiO_2 layer can avoid oxidation of the surface of a Si photoanode during oxygen evolution. Transparent metal oxide layers that block oxidative corrosion of efficient solar absorbers while permitting facile hole transport from the semiconductor to the overlying water oxidation catalyst layer have since become the standard approach for photoelectrochemical hydrogen synthesis. For Si photoanodes, the most favorable combination of photovoltage and photocurrent during water splitting has been achieved using thin ALD- TiO_2 protection layers on a buried p-n junction. However, a buried homojunction electrode has several drawbacks compared to a simpler metal-insulator-semiconductor (MIS) Schottky junction. We have investigated interface modification by post-gate annealing to boost the performance of MIS Schottky silicon photoanodes. This presentation will summarize promising approaches for simultaneously achieving high performance and stability of silicon photoanodes for water splitting, and the extent to which they can be generalized to other semiconductor systems.

4:45 PM

(EMA-S2-016-2017) High Throughput Atomic Layer Deposition: Interfacial Engineering at Scale (Invited)

J. Trevey^{*1}; D. King¹; A. Dameron¹; P. Lichty¹; 1. Forge Nano, USA

The benefits of Atomic Layer Deposition (ALD) have been widely demonstrated as a disruptive technology in numerous scientific fields ranging from semiconductor and energy storage devices to less conventional applications such as advanced ceramics, coated metal powders and more. With a history dating back to the 1970's there are many examples that highlight the step-function improvements that can be imparted to materials by ALD. For example, it can practically be taken for granted that most ‘smart’ devices are now fabricated using at least one ALD process or ALD coated component. However, while ALD in the semiconductor industry has seen explosive growth over the past decade, ALD on particles has yet to mature beyond bench-top equipment and systems. This lack of growth is a direct result of the excessive cost to perform particle ALD, as it has historically been a time and labor intensive process. At Forge Nano, we recognized the stranded nature of the particle ALD process, and addressed it by developing and patenting a new method for ALD known as High Throughput ALD. Our High Throughput ALD process has demonstrated the capability to meet both cost and performance targets of leading OEMs and raw material manufacturers in a variety of industries, with process intensification efforts currently underway to install systems capable of producing hundreds of tons of materials per year.

5:15 PM

(EMA-S2-017-2017) Structure and Photophysics of Surface Bound Molecular Species Stabilized with Sub-Nanometer Oxide Coatings for Electrochemical Devices

M. Losego^{*1}; B. Piercy¹; J. Song²; T. Lian²; 1. Georgia Institute of Technology, USA; 2. Emory University, USA

Molecularly sensitized devices that rely on surface bound molecules to impart functionality are keenly susceptible to device degradation via hydrolysis of anchor group chemistries and subsequent molecule

detachment. Examples include dye sensitized solar cells and electrolyzers with molecular catalysts. Recently, atomic layer deposition (ALD) of sub-nanometer oxide films “on top of” these functional molecules has proven effective in drastically improving long term device stability. This talk will highlight new understanding of how ALD affects the physical and chemical structure of these surface-bound molecules and the photophysical effects on electron transfer dynamics. New experiments using sum frequency generation to probe the orientation of surface-bound molecules before and after ALD will be discussed. Pico-second transient absorption spectroscopy studies revealing changes in charge injection rates as a function of ALD layer thickness and chemistry will also be presented. These studies provide further insights into the rational design of using ALD encapsulation as a means to stabilize molecular attachment while not degrading functional performance.

5:30 PM

(EMA-S2-018-2017) Unravelling Small-Polaron Transport in Bismuth Vanadate Photoelectrodes (Invited)

A. J. Rettie^{*1}; I. Argonne National Lab, USA

Bismuth vanadate (BiVO_4 , BVO) has emerged as a champion photoanode material for water splitting, but fundamental studies of this material are lacking. Electronic transport studies are especially uncommon, likely due to difficulties in synthesizing high quality samples and measuring high resistivity, low carrier mobility materials. Recently, we reported the synthesis of both undoped and tungsten doped BVO single crystals using the floating zone technique. We showed that electrons in this material move via thermally activated small polaron hopping transport between 250 and 400 K, and that the AC Hall mobility is low at room temperature: $\sim 0.2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. Unlike conventional, wide-band semiconductors, in small-polaron conductors the Hall and drift mobility may be vastly different. To determine a true drift mobility, the conductivity, Seebeck coefficient and AC Hall effect were measured in these crystals as functions of temperature and orientation. Furthermore, using small polaron theory we were able to map out the electronic structure of this material and generalize procedures for studying photoelectrodes that host small polarons.

S5: Energy Sustainable Optoelectronics and Magneto-electronics

Materials for Optoelectronics and Electro-Optics II

Room: Mediterranean C

Session Chairs: Jennifer Andrew, University of Florida; Jian Shi, Rensselaer Polytechnic Institute

2:00 PM

(EMA-S5-006-2017) Point defects and nanoscale chemistry in ultra wide band gap semiconductors (Invited)

J. Hwang^{*1}; 1. Ohio State University, USA

Establishing the structure-property relationship at the atomic to nanoscale is required to achieve high-performance and long-term stability of materials for energy and functional applications. We use novel quantitative characterization techniques in scanning transmission electron microscopy (STEM) to precisely quantify the atomic scale point defects and nanoscale chemical fluctuation in ultrawide band gap (UWBG) materials. UWBG semiconductors, such as AlGaIn and $\beta\text{-Ga}_2\text{O}_3$, open a new generation of devices for efficient UV emission and high power applications with their band gap up to 6.2 eV. With unmatched spatial resolution and precision of our technique, we examine the nanoscale chemical fluctuation between Al and Ga may alter local electronic structure in AlGaIn , and the point defects in $\beta\text{-Ga}_2\text{O}_3$ that may directly relate to the band gap and doping properties of the material. We will also discuss the state-of-the-art computational modeling of electron microscopy, which

provides new understanding of the electron channeling effect in STEM that can uncover the detailed information about point defects and nanoscale chemistry.

2:30 PM

(EMA-S5-007-2017) Van der Waals Epitaxy of Halide Perovskites

Y. Wang^{*1}; Y. Shi¹; J. Shi¹; 1. Rensselaer Polytechnic Institute, USA

The emergence of hybrid organic-inorganic halide perovskites has been widely recognized as a huge boost to the existing semiconductor family, enabling an upsurge of device performance in photovoltaic field which soon proceeds to the electro-optics and optoelectronics like photo detector and lasers. The growth of high quality single crystalline thin film lies in the core of the applications, either for exploring the intrinsic material physics or device engineering. By Van der Waals (VDW) epitaxy, we address a possible solution to the problem and realized single crystalline perovskite thin film up to several tens of microns in lateral dimension and down to a few nanometers in thickness on muscovite mica substrate. By using chemical phase epitaxy, we achieved the epitaxial growth of both organic (MA based) and Inorganic (Cs based) perovskite with all halide elements. By understanding the Van der Waals growth mechanism, we are able to obtain different epitaxial morphologies including two dimensional square flakes, fractal dendrites and one dimensional rod network structure. Our epitaxial film also shows a long range thickness dependent band gap shift which may be partially attributed to VDW epitaxial strain effect, something previously thought to be negligible. Our study would be of significance for both developing halide perovskite growth methods and also the fundamental understanding of the VDW epitaxy of non-layered soft materials.

2:45 PM

(EMA-S5-008-2017) Lasing characteristics of perovskites thin film assisted by localized surface plasmon (Invited)

T. Lu¹; T. Kao¹; K. Hong¹; F. Chen¹; Y. Chou^{*1}; 1. National Chiao Tung University, Taiwan

Due to the extraordinary optical property, high efficiency absorption, large photoluminescence quantum efficiencies and low cost solution processes, organic-inorganic halide perovskite has attracted enormous researchers diving into perovskite solar, LED and sensor technology during in the past years. However, only few reports demonstrated organic-inorganic halide perovskite on to coherent source. Here we report on the fabrication and characteristics of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite thin film by a two-step low temperature solution process. We discovered that the formation of polycrystalline grain boundary provided a random scattering path for optical feedback, thus the system can achieve the laser operation at a proper excitation power. The lasing wavelengths altered by different halide wt% in perovskite was also investigated. Moreover, we found that by adding a silver thin film onto the perovskite thin film with a PMMA capping layer, the strong plasmon-exciton interaction between the Ag and perovskite films can significantly reduce the excitation power threshold by two orders of magnitude than that acquired in bare perovskite layers. The excellent optical characteristic, simple and low cost process exhibited by the organic-inorganic halide perovskite would be suitable for making practical coherent sources.

3:15 PM

(EMA-S5-009-2017) 3D and uniform mesoporous TiO_2 films for application in Dye-Sensitized Solar Cells (DSSCs)

N. Tasić^{*1}; Z. Marinković Stanojević¹; Z. Branković¹; U. Lacnjevac¹; M. Zunic²; G. Branković¹; 1. Institute for Multidisciplinary Research, University of Belgrade, Serbia, Serbia; 2. College of Engineering and Information Technology, University of Business and Technology, Saudi Arabia

Dye-sensitized solar cells (DSSCs) are widely investigated 3rd generation photovoltaics on a verge of reaching the conversion efficiency

of 15%. The core of a typical DSSC is its photoanode, consisting of mesoporous TiO_2 layer deposited onto transparent conducting substrate, and sensitized with the light harvesting dye. In this paper, we propose novel method for preparation of large surface area TiO_2 particles, which can be processed into photoanodic films with 3D spherical architectures or uniform mesoporous structures. The method includes sol-gel processing of Ti(IV) -isopropoxide in the presence of $\text{Na}_2\text{-EDTA}$ and Triton X100, followed by autoclaving of as prepared gels, and sonication of gels into doctor blade TiO_2 pastes. DSSCs were fabricated using as prepared films, commercially available Ru(II) -sensitizer and iodine-based electrolyte. The operating parameters of DSSCs were extracted from current density-voltage (J-V) characteristics. The charge transport phenomena were investigated by recording electrochemical impedance spectra (EIS) and open-circuit voltage decay (OCVD) curves. The cells with uniform structure exhibited excellent short-current density (J_{sc}) response, up to 11.7 mA cm^{-2} , with the average photo-to-current efficiency of 5.0%, while the best photovoltaic response of cells with spherical architectures was 3.2%.

Magnetoelectrics and Multiferroics

Room: Mediterranean C

Session Chair: Jiamian Hu, University of Wisconsin, Madison

4:00 PM

(EMA-S5-010-2017) Multiferroism and Colossal Magneto-Capacitance of La modified M-type Lead Hexaferrite

G. Tan^{*1}; H. Sheng¹; W. Li¹; Y. Huang¹; 1. Wuhan University of Technology, China

Multiferroic materials with such magnetoelectric properties that are comparable to the useful ferroelectrics and ferromagnets are exceedingly rare. We report here on integration of ferroelectricity and ferromagnetism in a M-hexaferrite ($\text{La}_{0.2}\text{Pb}_{0.7}\text{Fe}_{12}\text{O}_{19}$), which simultaneously exhibits colossal magnetocapacitance effect. The coexistence of the off-centered FeO_6 octahedron and electron spins in partially filled Fe 3d or La 3f orbits is supposed to be responsible for emergence of mutually exclusive electric and magnetic orders. Five magnetoelectric phases and boundaries have been built up by the permeability profile. By applying a magnetic field (B), the capacity or dielectric constant demonstrates giant oscillations, whose maximum amplitude exceeds $1.90 \times 10^5\%$ at 80 Hz. The huge oscillations are associated with the variable component and orientation of the cycloid conic spins at the boundaries between two neighboring magnetic phases, where the cycloid cone axes align themselves parallel or reversal parallel to the direction of B field. Thus the dielectric constants are systematically enhanced to reach a giant value of ± 58270 or -84866 due to the great promotion of spin-current induced polarization.

4:15 PM

(EMA-S5-011-2017) Planar Defects in Magnetoelectric Cr_2O_3 Thin Films on Sapphire (Invited)

C. Sun¹; A. Rath¹; Z. Song¹; M. Street²; W. Echtenkamp²; C. Binek²; P. Voyles^{*1}; 1. University of Wisconsin-Madison, USA; 2. University of Nebraska, Lincoln, USA

Voltage-controlled switching of a magnetic layer via exchange bias coupling to the boundary magnetization of magnetoelectric Cr_2O_3 offers a promising avenue to low-power, voltage-controlled spintronic devices. Scaling and integration of Cr_2O_3 -based devices requires Cr_2O_3 thin films with magnetoelectric switching below the dielectric breakdown field, which has proven elusive. We have found characteristic planar boundaries along the c-axis in Cr_2O_3 thin films grown on sapphire by MBE, PLD, and IBD. These defects consist of a 60 deg. rotation of the Cr_2O_3 lattice about the c-axis plus a $\frac{1}{2}\langle 1120 \rangle$ antiphase shift in the plane of the film. Electron energy loss spectroscopy shows a prepeak on the O K-edge on the boundary that is not present in the perfect film. Density functional theory

from the experimentally-derived defect structure shows that the prepeak arises from a narrowing of the bandgap by almost 65% on the boundary. The decreased local bandgap means that the defects should exhibit a lower dielectric breakdown voltage than bulk Cr_2O_3 . Calculations also show ferromagnetic coupling of the Cr ions across the boundary, implying that the boundaries do not disturb the boundary magnetization responsible for magnetic switching. This work was supported by C-SPIN, a funded center of STARnet, a Semiconductor Research Corporation (SRC) program sponsored by MARCO and DARPA.

4:45 PM

(EMA-S5-012-2017) Fixed and Mobile Domain Walls in Multiferroics

J. Steffes^{*1}; P. Ashby⁴; L. Ye¹; Z. Thatcher¹; R. Ramesh³; J. Heron²; B. D. Huey¹; 1. University of Connecticut, USA; 2. University of Michigan, USA; 3. UC Berkeley, USA; 4. Lawrence Berkeley National Laboratory, USA

Multiferroic and ferroelectric materials are promising for a range of energy sustainable devices, including electro-magnetic sensors, non-volatile memory elements, piezotronics, and photovoltaics. Crucial to the functionality and reliability of these systems are the microstructure and stability of ferroelectric domains and domain walls. Using high speed PFM, switching and relaxation dynamics for BiFeO_3 are presented. The stability of nucleation sites, and especially domain walls, is directly assessed by cyclic poling, revealing clearly defect-coupled domain interfaces as well as mobile interfaces in a single field of view. Results are also presented for strained and relaxed functional thin films. Such investigations have profound implications for device scaling, functionality, and energy consumption.

5:00 PM

(EMA-S5-013-2017) Monitoring polar states of growing multiferroic heterostructures (Invited)

M. Trassin^{*1}; 1. ETH Zurich, Switzerland

In ferroelectric thin films, the polarization state, i. e. orientation and domain architecture, defines the macroscopic ferroelectric properties such as the switching dynamics. Ferroelectric domain engineering is in permanent evolution from the epitaxial strain tuning to the chemical control on interface atomic termination. Technology promising complex polar flux closure or vortices architecture have been recently demonstrated in ferroelectric heterostructures. However the mechanism involved in the formation of these complex polar states remains unexplored. The optical second harmonic generation process is an efficient and non-invasive tool for thin films ferroic properties probing. Here, we investigate the emergence of the ferroelectric polarization in ultra-thin ferroelectric and multiferroic films and monitor in situ the optical non-linear response of the film during the growth. We find that, the ferroelectric critical thickness and domain state can be measured in situ during the film deposition. Using a combination of epitaxial strain engineering and surface termination control in $(\text{BiFeO}_3/\text{SrRuO}_3)_n$ multilayers, we determine the BiFeO_3 net polarization orientation in each layer and in real-time, exempt from substrate contribution. Our work provides direct observation of ferroelectric states during the growth as well as new insights towards further control of ferroelectric based heterostructure.

5:30 PM

(EMA-S5-014-2017) Non-resonant Magnetoelectric Energy Harvester Utilizing Phase Transformation in Relaxor Ferroelectric Single Crystals

M. Staruch¹; R. Perez Moyet²; J. Stace²; A. Amin²; J. Restorff²; M. Wun-Fogle³; P. Finkel¹; 1. U.S. Naval Research Laboratory, USA; 2. Naval Undersea Warfare Center, USA; 3. Naval Surface Warfare Center Carderock, USA

Recent advances in phase transition transduction enabled the design of a non-resonant broadband mechanical energy harvester that is capable of delivering an energy density per cycle up to two orders of magnitude larger than resonant cantilever piezoelectric type generators. This was achieved in a [011] oriented and poled domain engineered relaxor ferroelectric single crystal, mechanically biased near a ferroelectric rhombohedral - ferroelectric orthorhombic phase transformation. At this critical point, a small variation in an input parameter, e.g., electrical, mechanical, or thermal will generate a large output due to the significant polarization change associated with the transition. This idea was extended to design a non-resonant, multi-domain magnetoelectric composite hybrid harvester comprised of a highly magnetostrictive $\text{Fe}_{81.4}\text{Ga}_{18.6}$ (Galfenol) alloy and lead indium niobate-lead magnesium niobate-lead titanate (PIN-PMN-PT) domain engineered relaxor ferroelectric single crystal. We have demonstrated high energy conversion in this magnetoelectric device by triggering the phase transition in the single crystal by a small ac magnetic field in a broad frequency range that is important for multi-domain hybrid energy harvesting devices.

S9: Interfaces in Microstructural Evolution: Structure, Properties, Anisotropy, and Motion

Impact of Interfacial Properties on Materials Properties and Processing

Room: Mediterranean A/B

Session Chairs: Rachel Zucker, University of California, Berkeley; Wolfgang Rheinheimer, Karlsruhe Institute of Technology

2:00 PM

(EMA-S9-008-2017) Electric Field Effects on Grain Boundary Formation and Grain Growth (Invited)

K. van Benthem¹; L. A. Hughes¹; W. Qin¹; 1. University of California, Davis, USA

The application of electric fields and current can enable the accelerated consolidation of ceramics during field assisted sintering. Prominent examples for such techniques are spark plasma sintering and flash sintering, which have both been employed for a wide variety of ceramics resulting in microstructures with unique macroscopic properties. A fundamental understanding of the atomic-scale mechanisms for both grain boundary formation and grain growth in the presence of electric fields has not been accomplished yet. To gain a deeper mechanistic understanding of the interplay between applied electric fields and emerging grain boundary structures we have synthesized bicrystals of SrTiO_3 in the presence and absence of electrostatic fields. Atomic resolution transmission electron microscopy techniques were used to study grain boundary core structures as a function of processing conditions. During flash sintering, however, electric fields and currents play an important role for densification and microstructure formation. Latest results on the effects of directional currents on the formation of texture in partially-stabilized ZrO_2 will be demonstrated. This work was funded by the Army Research Office under grants W911NF-12-1-0491 and W911NF-16-1-0364 (Program manager: Dr. David Stepp). LAH acknowledges financial support by an US National Science Foundation Graduate Research Fellowship under Grant No. 1148897.

2:30 PM

(EMA-S9-009-2017) A DoE Approach to Densifying Sodium Potassium Niobate (KNN) by Compositional Variation (Invited)

G. Corapcioglu¹; M. Papila²; M. A. Gulgun¹; 1. Sabanci University, Turkey; 2. Sabanci University, Turkey

As with all electroceramic KNN's dielectric properties are ultimately linked to the amount of porosity in the polycrystalline body. KNN suffers from serious densification problems because of alkali volatilization at relatively low temperatures and severe facetting during long term anneals. In order to densify KNN polycrystalline ceramics we combined two independent approaches: liquid phase densification and reactive sintering techniques. By using starting powders with compositions equi-distance from the ideal $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$ composition in mutually orthogonal compositional axes in proper proportions we mapped out the density contour of the $\text{Na}_2\text{O-K}_2\text{O-Nb}_2\text{O}_5$ phase diagram. KNN powers with compositional ranges of $(\text{K}_x\text{Na}_{1-x})_y\text{Nb}_{1-y}\text{O}_{3-\delta}$ $0.1 < y < 1.1$ ve $0.3 < x < 0.7$ were fabricated by solid-state synthesis method. Alkaline excess composition showed two step sintering behavior with a limited density compared to stoichiometric composition ($\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$). Sintering behavior of the powder compositions and the sintering behavior of the combinations of end members in orthogonal compositional directions in the phase diagram were investigated. Micro structural and micro-chemical investigations with the help of a TEM/EDS system helped understand the reactive sintering paths taken by different combinations to reach the maximum density in excess of 98% theoretical density by pressureless sintering.

3:00 PM

(EMA-S9-010-2017) Characterizing Grain Boundary Chemistry Effects on Strength using Single Boundary Measurements (Invited)

S. Dillon¹; 1. University of Illinois at Urbana-Champaign, USA

Many ceramics are known to embrittle with increasing grain size, relative to Hall-Petch extrapolations between fine grained and single crystal. As the grain size of materials like Al_2O_3 increase towards the macroscopic scale their strengths tend toward zero. Grain size effects are often considered as an isolated variable, but vastly different grain sizes must often be obtained from different annealing temperatures. However, in many oxides the atomic structures and chemistries of grain boundaries change with temperature. We hypothesize that this may be the dominant effect in the embrittlement of ceramics as a function of increased grain size. The hypothesis is difficult to prove by experimenting on polycrystals, because the counter argument is that flaw sensitivity is grain size dependent and thus an apparent embrittlement with increased grain size is fundamental to the particular system. To test our hypothesis, we perform nano-cantilever fracture toughness experiments on single grain boundaries fabricated from polycrystalline samples. We will present results for single grain boundary fracture measurements performed on different doped Al_2O_3 materials pre-annealed at different temperatures. The experiments are performed using in-situ TEM based nanomechanical testing. The results will be interpreted in context of what is known about grain boundary complexion transitions in this system.

4:00 PM

(EMA-S9-011-2017) Re-partitioning of dopants in intergranular regions to dictate grain growth behaviors in ceramics

H. Gu¹; 1. Shanghai University, China

In recent years, dopant segregation to grain boundary (GB) in ceramic systems was found to lead to GB facet-roughening transition, which developed into a GB complexion scheme to correlate directly with the abnormal grain growth (AGG). However, such GB "phase diagrams" raises important concerns: (a) first, intergranular glassy film (IGF) at roughened GB is common in ceramics but not in metals, hence the remarkable stability of IGF must have a bonding origin beyond counting or changing the foreign absorbate layers;

(b) second, such correlation of GB with AGG was only observed in Al_2O_3 , and not even in the original and model system Si_3N_4 ; (c) last but not the least, triple-grain pockets (TPs) accommodating large amount of dopants should not be ignored in either GB transitions or AGG. Here we report an analytical TEM study for dopants partitioning and re-partitioning behaviors at IGF by different GB facets in same ceramic systems, including Si_3N_4 and Al_2O_3 , occurred either before or during AGG process. These results indicate: (i) it is never fully true that there is a unique equilibrium IGF structure regardless different GB facets, in a given ceramic even the model system; (ii) similar IGF partitions or GB transitions could occur with and without triggering AGG; (iii) TP phase, especially glass composition, dictate GB/IGF compositions, their interactions dictate AGG behaviors.

4:15 PM

(EMA-S9-012-2017) Interfacial Processes in Cold Sintered Ceramics and Ceramic-Based Composites (Invited)

J. Guo^{*1}; H. Guo¹; A. Baker¹; S. Funahashi¹; M. Lanagan¹; C. Randall¹; I. The Pennsylvania State University, USA

The conventional thermal sintering process of ceramics is generally performed at high temperatures, typically ranging from several hundred to tens of hundreds of degrees Celsius, to enable the mass transport processes that allow the atoms, cations, or molecular groups to diffuse across the boundaries of adjoining particulates. Recently, we developed an extremely low temperature sintering technique for ceramics and ceramic-based composites, namely "Cold Sintering Process" (CSP). Basically CSP uses a transient aqueous environment to effect densification by a mediated dissolution-precipitation process. Since a transient liquid phase is involved in the Cold Sintering Process, it is important to understand the interfacial structures of Cold Sintered materials. A microwave dielectric ceramic is selected to show the grain boundary structures after CSP. Two diphasic composites (dielectric composite and semiconductor composite) are demonstrated to show the overall diversity of grain boundary design, including the design between micro-size and nano-size particles and the design between particles and fibers. With further understanding of interfacial processes, Cold Sintering would open up a new material design scheme impacting a wide variety of applications.

4:30 PM

(EMA-S9-013-2017) Interplay between phase boundary motion, diffusion and surface reaction in ion-insertion compounds (Invited)

M. Tang^{*1}; L. Hong¹; I. Rice University, USA

Phase transformations occur in many ion-insertion compounds for energy storage applications, in which phase boundary movement often limits (dis)charge kinetics. Compared to traditional materials, new phase transformation behavior emerges in ion-insertion compounds due to their open system nature. In particular, phase boundary motion can be influenced by surface reaction kinetics in addition to the well-known diffusion-limited and interface-reaction-limited mechanisms. In this work, we use mesoscale modeling to reveal the intricate interplay between ion diffusion and surface reaction in determining the phase transition kinetics, using olivine LiFePO_4 cathode as a prototypical model system. First, a new hybrid mode of phase growth, in which the phase boundary migration is controlled by bulk diffusion and surface reaction along different directions, is identified and explains recent observations from operando x-ray transmission microscopy. Second, we show that antisite defects, which strongly moderate Li diffusivity in LiFePO_4 , have very different effects on transformation rate in surface-reaction- and diffusion-limited regimes and may become desirable under certain circumstance. Our study suggests that facilitating phase boundary migration is an important consideration in tailoring particle morphology and defect content in ion-insertion compounds for improved performance.

5:00 PM

(EMA-S9-014-2017) Interface Stoichiometry and Evolution During Electrical Degradation of Barium Titanate

N. Creange^{*1}; M. J. Cabral¹; E. C. Dickey¹; I. North Carolina State University, USA

Resistance degradation has been widely studied in SrTiO_3 , but less is known about the mechanisms driving BaTiO_3 degradation, especially in the ferroelectric phase. During electronic degradation, oxygen vacancies migrate towards the cathode creating an inhomogeneous distribution of ionic defects. By understanding the evolution of stoichiometry in near interface regions as a function of electric field, temperature, and time, we can evaluate the factors controlling degradation in the ferroelectric phase. In this work, BaTiO_3 single crystals were allowed to equilibrate at 900°C in an inert reducing atmosphere, forming doubly ionized oxygen vacancies and providing well-defined initial conditions for degradation. Electrical degradation was performed under the Curie temperature while applying 50V/cm and an increase in current over an order of magnitude was observed. The local defect chemistry of near interface regions of the cathode and anode were measured through TEM using a combination of EELS and AC STEM. After degradation, significant changes in the domain structure were viewed under polarized light. Furthermore, we observe the effect of stoichiometry on defect clustering and ordering in the cathode region.

S12: 5G Materials for the Millimeter Wave Revolution

5G Materials for the Millimeter Wave Revolution II

Room: Caribbean B

Session Chair: Nate Orloff, NIST

2:00 PM

(EMA-S12-007-2017) Dimensional Control of Complex Transition Metal Compounds: Insights From First Principles (Invited)

T. Birol^{*1}; I. University of Minnesota, USA

The fact that the dimensionality of transition metal compounds' crystal structures have a strong effect on their macroscopic properties is well known, but the microscopic mechanism by which this happens is not always obvious. First principles methods, such as Density Functional Theory or Dynamical Mean Field Theory, are capable of providing insight that can help uncover these mechanisms. In this talk, after discussing some examples of dimensional control, I will explain the microscopic mechanism behind the emergence of novel polar phases in SrTiO_3 Ruddlesden-Popper compounds, and clarify how the interfacial rumpling, only recently observed experimentally in these systems, is responsible of the dimensional reduction.

2:30 PM

(EMA-S12-008-2017) A Millimeter-Wave Testbed for 2D Materials Including Transition Metal Dichalcogenides and Graphene

N. Orloff^{*3}; C. J. Long³; A. Jackson¹; I. Hanemann²; C. Little²; P. Kabos³; S. Berweger⁴; E. Cobas⁴; T. Palomaki⁵; M. Keller³; J. C. Booth³; I. Purdue University, USA; 2. University of Colorado, USA; 3. National Institute of Science and Technology, USA; 4. Naval Research Laboratory, USA; 5. University of Washington, USA

Microscale devices that are capable of emitting and detecting higher frequencies are important for sources and receivers used in next generation mobile technologies. Graphene, with electron mobility as high as $200,000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, shows promise as tunable material that has a number of applications relevant to high frequency microdevices. Other examples include transition metal dichalcogenides, which

may have novel applications as millimeter wave transistors, power amplifiers, or even novel circuit elements. Here, we develop a 2D material testbed, where the 2D material is either placed or patterned as essentially resistors with different lengths on a gold coplanar waveguide. Once the devices were fabricated, we developed a microwave measurement technique to characterize the materials behavior up to 110 GHz, as a function of temperature and bias voltage. Corresponding finite element simulations of the resistor-like geometry are also discussed to extract the material properties. Finally, we propose some potential device applications of these novel material systems.

2:45 PM

(EMA-S12-009-2017) Optically derived high spectral purity electronic signals from RF to W Band (Invited)

F. Quinlan^{*1}; T. Fortier¹; S. Diddams¹; 1. National Institute of Standards and Technology, USA

As the demands for low phase noise in applications such as radar, high-speed signal processing, precision microwave spectroscopy, and novel material metrology become more stringent, it is becoming increasingly difficult to meet system requirements with traditional electronic oscillators. Optical resonators can provide extremely high quality factors, in some cases exceeding 10^{11} , enabling highly frequency-stable and spectrally pure optical frequency references. In this talk, we will review the optical frequency division technique, by which the unparalleled stability of optical references is transferred to the RF, microwave, and millimeter-wave domains. Fractional frequency stability $< 10^{-15}$ for 10 GHz signal generation has been achieved, accompanied by noise floors approaching -180 dBc/Hz. Methods for realizing sub-millihertz tuning across RF, microwave, and millimeter-wave domains while maintaining fractional stability $\sim 10^{-15}$ will also be discussed.

3:45 PM

(EMA-S12-010-2017) Extending Transparency of Conductive Oxides into low THz and THz Spectrum (Growth and Characterization) (Invited)

D. Shreiber^{*1}; M. P. Ivill¹; M. W. Cole²; 1. US Army Research Laboratory, USA; 2. Central New Mexico College, Univ. of New Mexico, USA

Important challenges need to be addressed in order to bring the development of the 5G technology to the next level of readiness. One of them is significantly higher levels of the signal attenuation in the air in comparison with the 4G range of frequencies. Tunable complex oxide thin films are considered prime candidates to be utilized in the new generation of 5G components such as phase shifters, filters etc. The dielectric properties of these thin films can be tuned by applying a simple electrical bias. However, addition of bias electrodes to the system will contribute to additional attenuation losses in 5G components and some characterization devices proposed for the materials at 5G frequencies. A large body of work has been dedicated to conductive oxides, such as $\text{In}_2\text{O}_3\text{Sn}$ (ITO) or Sr_2RuO_4 (SRO) that are transparent at optical frequencies. This presentation will discuss growth approach and characterization of these conductive oxide thin films that help to extend their transparency into THz range of the radiation spectrum. This approach will make them to be very appealing candidates to be used in future 5G components.

4:00 PM

(EMA-S12-011-2017) Nickel Zinc-based Ferrite Thick Films Created via Tape Casting Method for Wide-bandwidth Conformal Antennae

T. Kittel^{*1}; G. Naderi¹; J. Schwartz¹; 1. North Carolina State University, USA

Nickel zinc ferrite ($\text{Ni}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$ (NZF)) and nickel zinc cobalt ferrite ($\text{Ni}_{0.19}\text{Zn}_{0.28}\text{Co}_{0.03}\text{Fe}_{2.5}\text{O}_4$ (NZCF)) are interesting materials for high-frequency wide-bandwidth antennae applications. A primary challenge in developing these materials for antennae applications is

obtaining the desired properties at a technologically relevant scale. Here, we present a method for creating NZF and NZCF large-area thick films by utilizing a tape casting system. In this study, different processing conditions are examined including sintering temperature, heating rate, and total sintering time. Scanning electron microscopy is used to study the changes in density, thickness, microstructure, and grain size with processing conditions. Variations in crystallographic texture are studied using X-Ray Diffraction. Magnetization behavior, including saturation magnetization and coercivity, is characterized using vibrating superconducting quantum interference device magnetometer. A short and open microstrip cavity is used to measure permeability and permittivity across microwave frequencies. Relationships between processing conditions and magnetic properties were found. For instance, relative permeability was found to increase with decreasing sintering time. Approaches to bonding films to substrates and creating thicker films via stacking of tape cast films are also explored.

4:15 PM

(EMA-S12-012-2017) Ultralow temperature cofiring ceramic materials for LTCC applications (Invited)

H. Wang^{*1}; 1. Xi'an Jiaotong University, China

With the rapid development of wireless hand-held devices, the needs for passive component devices working in microwave range with enhanced reliability, miniaturization and electrical performance are increasing fast. Low temperature cofiring ceramic (LTCC) provides one of good solutions for integrating the passive components as a functional module for microwave applications. Novel dielectric ceramics with the sintering temperature lower to 400°C to 600°C have been systematically investigated. The mechanism of microwave dielectric response was studied and the contribution of intrinsic and extrinsic dielectric loss was revealed. Ion substitutions as well as the biphasic composites were used to tailor the dielectric properties effectively. Prototype LTCC devices have been demonstrated.

S13: Mesoscale Phenomena in Ceramic Materials, Nano- and Microstructures

Multiscale Modeling of Mesoscopic and Interfacial Phenomena (Joint session with Symposium 10)

Room: Coral A

Session Chairs: Paul Evans, University of Wisconsin; Marty Gregg, Queens University Belfast

2:00 PM

(EMA-S13-006-2017) Predicting the coevolution of microstructure and properties in ceramic materials with the MOOSE framework (Invited)

M. R. Tonks^{*1}; I. Greenquist¹; F. Hilty¹; M. Sessim¹; J. Hirschhorn¹; 1. Pennsylvania State University, USA

The underlying microstructure of a ceramic material has a significant impact on the material's properties. Thus, the evolution of the microstructure modifies the properties, changing the performance. Modeling and simulation at the mesoscale can play an important role in predicting the evolution of the microstructure and the resultant change in properties. The Multiphysics Object Oriented Simulation Environment (MOOSE) is an open source finite element based simulation framework that comes with powerful modules for modeling microstructure evolution and estimating the effective properties of a given microstructure. In this presentation, I will highlight four areas in which MOOSE is being used to simulate the behavior of ceramics: fabrication using sintering, grain growth, phase transformation, and thermal transport.

2:30 PM

(EMA-S13-007-2017) Ferret: An open-source code for simulating materials thermodynamics at mesoscale

J. Mangeri¹; K. C. Pitike²; L. Kuna¹; A. Jokisaari³; P. S. Alpay²; O. Heinonen⁴; S. Nakhmanson^{*2}; 1. University of Connecticut, USA; 2. University of Connecticut, USA; 3. Northwestern University, USA; 4. Argonne National Lab, USA

Ferret is an open-source highly scalable real-space finite-element-method (FEM) based code for simulating transitional behavior of materials systems with coupled physical properties at mesoscale. This code is built on MOOSE, Multiphysics Object Oriented Simulation Environment, and is being developed by a team of collaborators at the University of Connecticut and Argonne National Laboratory. In this presentation we provide an overview of the code technical features and highlight some of its applications. These applications include (a) evaluations of size- and microstructure-dependent elastic and optical properties of core-shell nanoparticles, including Zn/ZnO and ZnO/TiO₂ core/shell material combinations; (b) modeling of the influence of shape, size and elastic distortions of monolithic ZnO and Zn/ZnO core/shell nanowires on their optical properties; (c) studies of the properties and domain-wall dynamics in perovskite-ferroelectric films, nanowires and nanoridges, and (d) investigation of transitional behavior and topological phases in ferroelectric nanoinclusions embedded in a dielectric matrix. Finally, we showcase the results of our efforts to parameterize the coarse-grained thermodynamical expressions used by Ferret with the help of first-principles simulations, including different strategies for fitting Landau-type energy functionals for perovskite structures.

2:45 PM

(EMA-S13-008-2017) Temperature-induced ferroelectric phase transition in ABO₃ perovskites: A Wang-Landau-DFT approach

S. F. Yuk^{*2}; K. C. Pitike²; S. Nakhmanson²; M. Eisenbach³; Y. W. Li³; V. R. Cooper¹; 1. Oak Ridge National Lab, USA; 2. University of Connecticut, USA; 3. Oak Ridge National Lab, USA

ABO₃ perovskite oxides exhibit a wide range of dielectric and piezoelectric responses due to variations in possible A- and B-site metal cations as well as temperature- and pressure-dependent accessible phase transitions. While first principles methods have excelled at predicting ground state properties, accurate evaluation of ferroelectric phase transitions is a challenging task with the estimated phase transition temperatures often being significantly lower than the experimental values. These failures are coupled to errors in density functional theory (DFT), such as the choice of exchange and correlation (XC) functional, as well as the limitation in simulations of temperature-dependent properties. As our first step to tackling this issue, we have performed Wang-Landau simulations using DFT energies obtained with different XC functionals to explore the role that this choice has on the temperature-induced phase transitions of prototypical perovskites. These results give us insights into proper approaches for modeling these materials. Furthermore, this method is general and therefore has the further potential for assisting in the acceleration of materials design and understanding; with broad applicability across a wide range of material systems. Research was sponsored by the US DOE, Office of Science, BES, MSED and Early Career Research Programs and used resources at NERSC and OLCF.

3:00 PM

(EMA-S13-009-2017) First-principles-based Landau energy functionals for perovskite ferroelectrics

K. C. Pitike^{*1}; N. Gadigi²; J. Mangeri³; V. R. Cooper⁴; S. Nakhmanson¹; 1. University of Connecticut, USA; 2. University of Connecticut, USA; 3. University of Connecticut, USA; 4. Oak Ridge National Laboratory, USA

ABO₃ perovskite-oxide ferroelectrics are well known for their useful functional properties. These materials, as well as their solid solutions, exhibit rich phase diagrams that can be exploited, e.g., to

obtain large piezoelectric and dielectric responses. Mesoscale-level investigations of their behavior usually utilize Landau phenomenological theory, where the system energy functional is represented by a polynomial expansion in powers of polarization and strain that is parameterized from experimental data. In this project, we present an approach for fitting the Landau functionals for perovskite ferroelectrics directly from first principles simulations with the help of statistical and machine learning tools. Initial data sets are created by computing the energies for a wide range of possible structural configurations involving polar and elastic distortions with standard density-functional theory (DFT) codes. A small fraction of this data is then processed by supervised machine learning algorithms to train a Landau-style polynomial model that can predict the system energies to within 20 meV of the DFT results.

3:45 PM

(EMA-S13-010-2017) Intrinsic size effects and topological phase transformations in ferroelectric nanoinclusions embedded in a dielectric matrix (Invited)

J. Mangeri^{*1}; Y. Espinal²; A. Jokisaari³; P. S. Alpay²; S. Nakhmanson²; O. Heinonen⁴; 1. University of Connecticut, USA; 2. University of Connecticut, USA; 3. Northwestern University, USA; 4. Argonne National Lab, USA

Self-assembled ferroelectric-nanoinclusion / dielectric-matrix composites with tuneable properties can be employed in a variety of next-generation electronic devices. In this investigation, we utilize a thermodynamic Landau-Ginzburg approach to study size dependence of the emergent functional behavior of spherical PbTiO₃ and BaTiO₃ nanoparticles embedded in a dielectric medium. We show that the choice of both ferroelectric-inclusion and surrounding-matrix materials strongly affects the emerging polarization-vector pattern. Specifically, a monodomain phase of PbTiO₃ is supported below some critical nanoinclusion diameter when combined with a high- κ dielectric medium. Above this critical diameter, a vortex-like texture occurs in both PbTiO₃ and BaTiO₃, while for even larger inclusion sizes a polydomain phase is formed. Furthermore, when an external electric field is applied to the composite, for certain nanoinclusion sizes we observe switching between monodomain and vortex states, which in turn produces hysteresis curves exhibiting both ferroelectric and antiferroelectric features. Finally, we will also discuss the influence of elastic coupling with the matrix, as well as the choice of model polar gradient energy coefficients, on the composite functional behavior and compare these results to a number of previous experimental and theoretical studies.

4:15 PM

(EMA-S13-011-2017) Kinetic Poisson-Cahn Model of Defect Segregation Near Grain Boundaries During Thermal Annealing in Oxygen-Conducting Solid Electrolytes

X. Tong^{*1}; D. S. Mebane¹; 1. West Virginia University, USA

Aliovalently-doped fluorites are good electrolytes for solid oxide fuel cells due to the ionic conductivity introduced by oxygen vacancies. The total conductivity of these materials, however, is restricted by the presence of grain boundaries. Defect segregation near grain boundaries significantly contributes to this phenomenon. Past research has shown the importance of thermal processing history on ionic conductivities; a deeper understanding of the non-equilibrium distribution of dopant cations established during thermal processing could guide the design of electrolytes with more favorable grain boundary conductivities. Taking CeO₂-Gd₂O₃ as a model system, a kinetic model is developed to simulate defect segregation during thermal annealing based on the Poisson-Cahn model for defect segregation in both dilute and concentrated solid solutions. Results reveal the systematic evolution of non-equilibrium dopant distribution near a grain boundary for solid solutions with 20%, 1% and 0.1% dopant cation concentration. The amount of time for the dopant profile to approach equilibrium increases from a scale of a fraction of a second at 1300°C to more than 15 hours at 900°C.

4:30 PM

(EMA-S13-012-2017) The Poisson-Cahn space charge theory for concentrated solid electrolytes (Invited)

D. S. Mebane^{*1}; 1. West Virginia University, USA

A steady stream of new experimental results has made it increasingly impossible to ignore the failure of conventional, dilute-case space charge theories (most prominently, Gouy-Chapman and Mott-Schottky theories) to describe the observed picture of space charge zones nanometers wide and co-accumulated in concentrated solid solutions. The "Poisson-Cahn" theory addresses these experimental findings in concentrated systems while remaining fully consistent with the dilute theories at appropriately low solute concentrations. Poisson-Cahn replaces the Boltzmann electrochemical potential in the Poisson-Boltzmann theory with a more general expression derived for concentrated, inhomogeneous mixtures; this inhomogeneous "Cahn" chemical potential was widely successful in its description of spinodal decomposition in alloys. The theory will be introduced, to include an illustration of its relationship with earlier theories. The ability of the theory to both qualitatively and quantitatively reproduce experimental results will be demonstrated.

S14: Multifunctional Nanocomposites

Synthesis of Functional Heterostructures

Room: Caribbean C

Session Chair: Erik Enriquez, Los Alamos National Lab

2:00 PM

(EMA-S14-007-2017) Mapping growth windows in strongly-correlated quaternary perovskite oxide systems by hybrid molecular beam epitaxy (Invited)

M. Brahele^{*1}; L. Zhang¹; J. Lapano¹; H. Zhang¹; R. Engel-Herbert¹; 1. Pennsylvania State University, USA

Metal-insulator transitions, high-temperature superconductivity and colossal magnetoresistance represent a few of the many phenomena that emerge in the solid solution $A'_{1-x}A_xBO_3$. Growing these in thin film form is, however, a challenge due to the precise control required for the composition, x , as well as the stoichiometry $(A+A')\colon B$. The hybrid metal-organic molecular beam epitaxy (hMBE) technique has been shown to exactly control stoichiometry, but requires understanding how to interpolate the growth conditions between the end members $A'BO_3$ and ABO_3 . Using the example of $La_{1-x}Sr_xVO_3$, the two-dimensional growth parameter space spanned by the flux of the metal-organic precursor vanadium oxytriisopropoxide and composition, x , can be mapped quickly with a single calibration sample using in situ reflection high-energy electron (RHEED), which is corroborated by X-ray diffraction and atomic force microscopy. This strategy enables the growth of stoichiometric perovskite oxide films with random A-site cation mixing. In particular, at the quantum critical point that separates the Mott-insulator ($LaVO_3$) from a strongly-correlated Fermi-liquid ($SrVO_3$) this ability to produce ultrahigh quality films allows the novel competition between disorder-effects and electron-electron interactions to be revealed. Supported by the Dept. of Energy (DE-SC0012375).

2:30 PM

(EMA-S14-008-2017) On the Growth of Epitaxial $SrCoO_x$ Phases During Oxide Molecular Beam Epitaxy (Invited)

D. Fong^{*1}; T. K. Andersen²; S. Cook²; 1. Argonne National Lab, USA; 2. Northwestern University, USA

Depending on the oxygen stoichiometry, $SrCoO_x$ can vary from $SrCoO_{2.5}$ (the brownmillerite phase) to $SrCoO_3$ (the perovskite phase) or phases in between. Using in-situ X-ray Oxide Molecular Beam Epitaxy (XOMBE), we explore the stability of these phases as functions of oxygen / ozone pressure, temperature, growth rate, and strain state. Through a combination of synchrotron X-ray scattering

and absorption spectroscopy techniques, we find that despite the appearance of different crystal structures, there is considerable variability in the Co oxidation state and thus oxygen stoichiometry. Unsurprisingly, strain state is the most important factor in determining the phase, but we find that the ozone pressure can be used to generate mixed phase, epitaxial composites.

3:00 PM

(EMA-S14-009-2017) Metal-Insulator Transition, Charge Compensation, and Mobility-Limiting Scattering Mechanisms in MBE Grown La-doped $BaSnO_3$ Films and Heterostructures (Invited)

A. Prakash¹; P. Xu¹; B. Jalan^{*1}; 1. University of Minnesota, USA

We will present the electronic transport properties of La-doped $BaSnO_3$. Carrier density and room-temperature mobility were used to optimize the buffer and active layer thicknesses. An optimum thickness of 124 nm each was determined. Films were grown with different dopant concentrations between $5 \times 10^{18} \text{ cm}^{-3}$ and $1 \times 10^{21} \text{ cm}^{-3}$. A maximum room-temperature mobility of $124 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ was observed at a carrier density of $4 \times 10^{20} \text{ cm}^{-3}$, which is amongst the highest reported mobility in La-doped $BaSnO_3$ films on $SrTiO_3$ substrate reported so far in literature. A metal-to-insulator transition (MIT) was observed at a resistivity value between $0.03 \text{ } \Omega \text{ cm} - 0.06 \text{ } \Omega \text{ cm}$ consistent with Mott's prediction. This MIT occurred at a carrier density between $5 \times 10^{18} \text{ cm}^{-3}$ and $1 \times 10^{19} \text{ cm}^{-3}$, which is higher than the expected value, indicating the role of compensating defects. A detailed study of temperature dependent mobility indicated different scattering mechanism at play at different temperature range and different carrier concentration. These will be discussed in the framework of further improving the room-temperature mobility in thin films of $BaSnO_3$.

Multifunctional Nanocomposites: The Interface I

Room: Caribbean C

Session Chair: Dillon Fong, Argonne National Lab

4:00 PM

(EMA-S14-010-2017) Self-Assembled Magnetic Metallic Nanopillars in Ceramic Matrix with Anisotropic Magnetic and Electrical Transport Properties

J. Huang^{*1}; Q. Su²; W. Zhang²; P. Lu³; F. Chen⁴; X. Zhang¹; J. MacManus-Driscoll⁵; A. Chen⁶; Q. Jia⁶; H. Wang¹; 1. Purdue University, USA; 2. Texas A&M University, USA; 3. Sandia National Laboratories, USA; 4. University of South Carolina, USA; 5. University of Cambridge, United Kingdom; 6. Los Alamos National Laboratory, USA

Ordered arrays of metallic nanopillars embedded in a ceramic matrix have recently attracted considerable interest for their multifunctionality in advanced devices. A number of hurdles need to be overcome for achieving practical devices, including selections of metal-ceramic combination, creation of tunable and ordered structure, and control of strain state. In this article, we demonstrate major advances to create such a fine nanoscale structure, i.e., epitaxial self-assembled vertically aligned metal-ceramic composite, in one-step growth using pulsed laser deposition. Tunable diameter and spacing of the nanopillars can be achieved by controlling the growth parameters such as deposition temperature. The magnetic metal-ceramic composite thin films demonstrate uniaxial anisotropic magnetic properties and enhanced coercivity compared to that of bulk metal. The system also presents unique anisotropic electrical transport properties under in-plane and out-of-plane directions. This work paves a new avenue to fabricate epitaxial metal-ceramic nanocomposites, which can simulate broader future explorations in nanocomposites with novel magnetic, optical, electrical, and catalytic properties.

4:15 PM

(EMA-S14-011-2017) Vertically aligned oxide heteroepitaxy films for fast oxygen ion transport at reduced temperature (Invited)

S. Lee^{*1}; J. MacManus-Driscoll²; 1. Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea; 2. University of Cambridge, United Kingdom

Oxygen ion transport in oxides has a wide spectrum of electrochemical functionalities, useful for potential energy applications such as solid oxide fuel cells (SOFCs). However, the current operation temperature of SOFCs is extremely high ($> 800^{\circ}\text{C}$) due to limited oxygen ion conductivity in oxide electrolytes and electrodes, resulting in several critical issues in SOFCs. Here, we will introduce vertically aligned oxide heteroepitaxy films, which show fast oxygen ion transport at much reduced temperature ($< 650^{\circ}\text{C}$). We design and create unique cell geometry of micrometer-thick epitaxial nanocomposite films, which include nanocolumns of either Sm-doped CeO_2 , Y-stabilized ZrO_2 , or SrZrO_3 . The ion conductivity of each nanocolumn is enhanced by several orders of magnitude compared to plain films, and is further improved by tensile strain in a vertical direction. Our successful heteroepitaxy of oxides will open the door to study the fundamental properties for potential energy applications and understand their intrinsic physics.

4:30 PM

(EMA-S14-012-2017) Termination control of magnetic order at a complex oxide interface (Invited)

K. Dorr^{*1}; 1. MLU Halle-Wittenberg, Germany

Atomically flat interfaces between ternary oxides have chemically different variants, depending on the terminating lattice planes of both oxides. The electronic interface state may fundamentally change with the interface termination, one prominent example being the $\text{LaAlO}_3/\text{SrTiO}_3$ interface with a two-dimensional electron system found for one of the two possible terminations. Well-defined terminations have yet rarely been demonstrated for oxide films of ABO_3 type (with metals A, B), but have become accessible recently. In my talk, I discuss a strategy of thin film growth and interface characterization applied to fabricate the $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ - SrRuO_3 interface with controlled terminations. X-ray magnetic circular dichroism measurements enabled tracking the elemental hysteresis curves of Ru and Mn and revealed fundamentally different magnetic coupling and switching depending on the interface termination. Ultra-strong antiferromagnetic coupling between the ferromagnets occurs at the MnO_2 - SrO interface, resulting in a controllable non-collinear magnetic structure in the SrRuO_3 layer. The RuO_2 - $\text{La}_{0.7}\text{Sr}_{0.3}\text{O}$ interface shows moderate magnetic coupling and exchange-bias-like behavior, in agreement with density functional calculations. Our results demonstrate a pathway for efficient termination control of magnetic coupling across complex oxide interfaces.

5:00 PM

(EMA-S14-013-2017) Interfacial Charge Engineering for Enhanced Ferroelectric-Control of Strongly Correlated Oxides

X. Chen¹; X. Zhang¹; M. A. Koton²; H. Chen³; Z. Xiao¹; L. Zhang¹; J. E. Shield²; P. Dowben¹; X. Hong^{*1}; 1. University of Nebraska-Lincoln, USA; 2. University of Nebraska-Lincoln, USA; 3. New York University-Shanghai, China

The energy competition of charge itineracy with the strong electron-electron and electron-phonon couplings in strongly correlated oxides make their electronic properties highly sensitive to the manipulation of the charge degree of freedom. In this work, we employ the interfacial charge transfer effect between two strongly correlated oxides, $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{NiO}_3$ (SNNO) and $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (LSMO), to realize a giant enhancement in the performance of ferroelectric-controlled Mott field effect transistors (FETs). By switching the polarization field of a ferroelectric $\text{Pb}(\text{Zr,Ti})\text{O}_3$ gate, we have induced nonvolatile resistance modulation in Mott FETs with ultrathin SNNO and SNNO/LSMO heterostructure channels. For both

channel systems, the magnitude of the field effect increases significantly with decreasing channel thickness. However, for the same total channel thickness, the room temperature resistance switching ratio is up to two orders of magnitude higher in the SNNO/LSMO channels, which is attributed to the carrier density attenuation in SNNO due to the charge transfer effect at the interface with LSMO. First principles density functional theory calculations point to 0.1-0.2 electron/Mn transfer, which is confirmed by the XPS and XAS measurements. Our approach can be utilized to tailor the properties of composite multiferroics for developing novel nanoelectronic and spintronic applications.

S15: Superconducting Materials and Applications**New Superconducting Materials and Phenomena II**

Room: Pacific

Session Chairs: Xianhui Chen, University of Science and Technology of China; Gang Wang, Institute of Physics, Chinese Academy of Sciences

2:00 PM

(EMA-S15-007-2017) Search for Topological Superconductivity in $\text{Sr}_x\text{Bi}_2\text{Se}_3$ (Invited)

H. Wen^{*1}; 1. Nanjing University, China

Topological superconductor is a very interesting and frontier topic in condensed matter physics. Despite the tremendous efforts in exploring the topological superconductivity, its presence is still under heavy debates. In this work, we report two progresses: (1) The surface Dirac electrons can be driven into Cooper pairs^[1], and (2) There is a two-fold symmetric superconductivity^[2] in $\text{Sr}_x\text{Bi}_2\text{Se}_3$. By measuring the scanning tunneling microscope/spectroscopy on $\text{Sr}_x\text{Bi}_2\text{Se}_3$, we find the full superconducting gaps without any in-gap density of states as expected theoretically for the bulk topological superconductivity. However, we find that the surface Dirac electrons will simultaneously condense into the superconducting state when the energy is smaller than the bulk superconducting gap. This vividly demonstrates how the surface Dirac electrons are driven into Cooper pairs. Furthermore, we measure the c-axis resistivity with the magnetic field rotating within the basal planes, and find clear evidence of two-fold superconductivity. The Laue diffraction measurements on these samples show that the maximum gap direction is either parallel or perpendicular to the main crystallographic axis. This observation is consistent with the theoretical prediction and strongly suggests that $\text{Sr}_x\text{Bi}_2\text{Se}_3$ is a topological superconductor. [1] Guan Du et al., arXiv.condmat:1604.08198. [2] Guan Du et al., arXiv.condmat:1607.06357.

2:30 PM

(EMA-S15-008-2017) Topological superconductor and Majorana fermions in the vortex (Invited)

J. Jia^{*1}; 1. Shanghai Jiao Tong University, China

Majorana fermion (MF) whose antiparticle is itself has been predicted in condensed matter systems. MFs can be used in fault-tolerant quantum computation relying on their non-Abelian braiding statistics, therefore, lots of efforts have been made to find them. Signatures of the MFs have been reported as zero energy modes in various systems. As predicted, MF in the vortex of topological superconductor appears as a zero energy mode with a cone like spatial distribution. Also, MF can induce spin selective Andreev reflection (SSAR), a novel magnetic property which can be used to detect the MFs. Here, I will show you that the $\text{Bi}_2\text{Te}_3/\text{NbSe}_2$ hetero-structure is an artificial topological superconductor and all the three features are observed for the MFs inside the vortices on the $\text{Bi}_2\text{Te}_3/\text{NbSe}_2$. Especially, by using spin-polarized scanning tunneling microscopy/spectroscopy (STM/STS), we observed the spin dependent tunneling

effect, which is a direct evidence for the SSAR from MFs, and fully supported by theoretical analyses. More importantly, all evidences are self-consistent. Our work provides definitive evidences of MFs and will stimulate the MFs research on their novel physical properties, hence a step towards their statistics and application in quantum computing.

3:00 PM

(EMA-S15-009-2017) Exploring unique electronic states at topological insulator-superconductor interfaces (Invited)

P. A. Folkes^{*2}; P. J. Taylor¹; C. Rong¹; B. Nichols¹; H. Hier¹; M. Neupane¹;
1. U.S. Army Research Laboratory, USA; 2. US Army Research Laboratory, USA

The recent theoretical prediction and experimental observation of topological insulators has stimulated intense research on proximity-induced topological superconductivity at topological insulator-superconductor interfaces which are predicted to host Majorana fermions. In this talk we present results of our research on materials and processing that will enable us to investigate the unique electronic states between topological insulators (TIs) and conventional / high-temperature superconductors. The objectives are: (1) molecular beam epitaxial (MBE) growth of PbSnTe and PbSnSe and verification that they are topological crystalline insulators (TCI); (2) MBE growth of 2D tin (stanene) and verification that it is a TI; and (3) growth and characterization of tin-based TI/superconductor heterostructures. The MBE growth and characterization of high-quality epitaxial TCI Pb_{0.5}Sn_{0.5}Te will be discussed. Thin layers of single crystal epitaxial semiconductor tin (a-Sn) were grown by MBE on CdTe substrates. X-ray diffraction and Raman scattering measurements confirm that the thin layers of a-Sn are slightly strained which supports theoretical prediction that a-Sn is a 3D TI. This is a prerequisite for the MBE growth of stanene. We have synthesized high temperature superconductor bismuth-strontium-calcium copper-oxide (Bi2212) substrates and achieved MBE growth of epitaxial PbSnTe on Bi2212 substrates.

4:00 PM

(EMA-S15-010-2017) Weyl nodes in noncentrosymmetric superconductor (Invited)

H. Weng^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

Weyl semimetal is a topological quantum state, which harbors topologically robust energy nodes with definite chirality formed by band crossing of nondegenerate bands in three-dimensional momentum space. The chiral Weyl nodes are close to chemical potential and contribute to the transport properties, such as negative magnetoresistivity due to "chiral anomaly". The nonmagnetic Weyl semimetal is noncentrosymmetric in order to have Rashba-like spin split to separate the chiral Weyl nodes. If superconducting coupling is further introduced into Weyl semimetal, the topological superconductor with p+ip pairing is expected and this will lead to realization of Majorana zero modes in vortex core or end boundary. In this talk, I will introduce our recent efforts in searching for superconducting Weyl semimetal.

4:30 PM

(EMA-S15-011-2017) Investigations of unconventional superconductivity under hydrostatic pressure conditions (Invited)

J. Cheng^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

The coexistence and competition between superconductivity and electronic orders, such as spin or charge density waves, have been a central issue in the unconventional superconductors. The application of hydrostatic pressure provides an effect and clean means to tuning the competitions of multiple electronic orders, allowing us not only to explore novel classes of unconventional superconductors near the pressure-induced magnetic quantum critical point, but also to reveal the underlying mechanisms of unconventional

superconductivity by elucidating the intimate relationship of superconductivity with other competing electronic orders. In this talk, I will present our recent effort on the investigations of unconventional superconductivity by utilizing the high-pressure approach: including (1) the discovery of superconductivity in CrAs and MnP near their pressure-induced helimagnetic quantum critical point [1, 2], (2) the construction of the most comprehensive T-P phase diagram of FeSe single crystal revealing implicitly the competing nature between high-T_c superconductivity and the long-range magnetic order [3], and (3) the observation of competition between superconductivity and the spin singlet state in Mo₅Sb₇ [4]. [1] W. Wu, et al., Nat. Comm. 5, 5508 (2014) [2] J.-G. Cheng, et al., PRL 114, 117001 (2015) [3] J. P. Sun, et al., Nat. Comm. 7, 12146 (2016) [4] G. Z. Ye, et al., Submitted (2016)

5:00 PM

(EMA-S15-012-2017) Molecular intercalated superconducting materials in iron compounds (Invited)

S. Jin^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

It is well established that the occurrence of superconductivity in iron pnictides is closely related to the tetragonal to orthorhombic structural and antiferromagnetic (AFM) phase transitions. It, however, has not been clear whether the same scenario is appropriate for iron chalcogenide counterparts due to the absence of parent compounds for the latter family of superconductors. Here, we report the synthesis and structure determination of two novel phases in ethylenediamine intercalated FeSe, one is tetragonal and the other orthorhombic in room temperature, which can be stabilized with neutral spacer layers. Both phases can be regarded as the parent compounds for superconductivity as they are non-superconducting (non-SC) in pristine form and superconducting (SC) with T_c up to 38K and 46K, respectively after Na doping, and the switch between SC and no-SC is reversible. Moreover, the two non-SC parent compounds show no evidence of long-range magnetic ordering down to 2K, only with dynamic spin fluctuations at low temperatures, suggesting that no competition between SC and AFM ordering.

Poster Session

Room: Atlantic/Arctic

5:30 PM

(EMA-P001-2017) Evolution of Brownmillerite Structure in SrCO_{2.5} Under Varying Molecular Beam Epitaxy Growth Conditions

T. K. Andersen^{*1}; S. Cook¹; H. Hong²; D. Fong³; L. D. Marks¹;
1. Northwestern University, USA; 2. Argonne National Lab, USA;
3. Argonne National Lab, USA

The Brownmillerite SrCoO_{2.5} (BM-SCO) is of interest for applications including solid-oxide fuel cells and batteries due to its high oxygen vacancy (V_o^{••}) concentration. This work focuses on determining the minimal film thickness to support ordered V_o^{••} structure in BM-SCO and formation of the SrCoO_x structure under varying growth environments - features important for applications where vacancy-induced functionality must be preserved. We employed in-situ x-ray oxide molecular beam epitaxy at Sector 33ID-E of the Advanced Photon Source for synthesis. Films were grown epitaxially on (001) LSAT and SrTiO₃ at 550°C and varying ozone gas pressure. After shuttered deposition of each SrO/CoO_{1.2} unit-cell via Sr and Co metals evaporated by Knudsen cells, the scattered intensity along the out-of-plane direction (00L) was measured using 8 keV x-rays. X-ray absorption near-edge spectroscopy at the Co K-edge were measured at 7.71 keV. From the 00L scattered intensity the BM-SCO structure can be observed after deposition of as few as 4-5 (SrO/CoO_{1.2}) unit-cells as evidenced by the characteristic half-order diffraction peaks. The Co K-edge energy shift increases with film thickness but the

oxidation state of Co quickly plateaus indicating that an interfacial region is very thin and high-quality BM-SCO films can be grown with thicknesses close to the periodic limit of their structure.

(EMA-P002-2017) Characterization of Solution-Based Exfoliated Nanosheets

K. G. Pachuta^{*1}; A. Sehrioglu¹; E. Pentzer²; 1. Case Western Reserve University, USA; 2. Case Western Reserve University, USA

The optimization and complete characterization of the delithiation and exfoliation of powders, Lithium Cobalt Oxide (LiCoO_2) and Lithium Nickel Manganese Cobalt Oxide ($\text{Li}[\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}]\text{O}_2$), to nanosheets was investigated. This process was achieved by the use of an aqueous solution-based chemistry route. Delithiation was achieved by treatment of the powder with hydrochloric acid (HCl). Exfoliation of the delithiated powder to nanosheets was completed via treatment with tetramethylammonium hydroxide (TMAOH). Optimization of the delithiation of the powders was accomplished by altering the frequency, duration, and concentration of HCl treatment. To optimize the nanosheet concentration and size, the particle size, the treatment of TMAOH, as well as the mechanical treatment employed after chemical modifications were altered. X-Ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD), Nitrogen/Oxygen/Hydrogen Determination (NOHD), Inductively Coupled Plasma–Optical Emission Spectroscopy (ICP-OES), and Ultraviolet/Visible Spectroscopy (UV/Vis) were the techniques implemented to fully characterize the delithiation and exfoliation to nanosheets.

(EMA-P003-2017) Optimizing Single Crystal Epitaxial $\text{Li}_{1-x}\text{La}_x\text{TiO}_3$ Growth on SrTiO_3 Substrate

E. Farghadany^{*1}; A. Sehrioglu¹; 1. Case Western Reserve University, USA

Solid state electrolytes are of interest to replace flammable liquid organic electrolytes due to safety issues. $\text{Li}_{1-x}\text{La}_x\text{TiO}_3$ (LLTO) is a perovskite complex oxide which shows high Li^+ ionic conductivity and very high transport number. Certain structural features in bulk LLTO like grain boundaries or domains due to ordering of A-site species where La ions limit vacancy mediated Li diffusion, cause a decrease in ionic conductivity. Epitaxially grown single crystal films are investigated to overcome such limitations and study the conduction mechanisms. LLTO films were grown by Pulse Laser Deposition (PLD) on SrTiO_3 substrates. Fluence of laser, pulse frequency, substrate temperature and partial pressure of oxygen in deposition atmosphere were the main parameters of the study to control the growth characteristics and rate of the film which was determined by in-situ RHEED. The structure and the thickness of the films were verified by X-ray diffraction and X-ray reflectivity, respectively. Transmission electron microscopy was utilized to characterize detailed structural features of the films.

(EMA-P004-2017) Processing and Performance of Sintered Intercalation Oxide Cathodes for All-Solid-State Structural Lithium Ion Batteries

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All-solid-state structural lithium ion batteries serve as both structural load-bearing components and as electrical energy storage devices to achieve system level weight savings in aerospace and other transportation applications. This multifunctional design goal is critical for the realization of next generation hybrid or all-electric propulsion systems. Additionally, transitioning to solid state technology improves upon battery safety from previous volatile architectures. This research established baseline solid state processing conditions and performance benchmarks for intercalation-type layered oxide materials for multifunctional application. Under consideration were lithium cobalt oxide and lithium nickel manganese cobalt oxide. Pertinent characteristics such as electrical conductivity, strength, chemical stability, and microstructure were characterized for future application in all-solid-state structural battery cathodes. The study

includes characterization by XRD, ICP, SEM, ring-on-ring mechanical testing, and electrical impedance spectroscopy to elucidate optimal processing parameters, material characteristics, and multifunctional performance benchmarks. These findings provide initial conditions for implementing existing cathode materials in load bearing applications.

(EMA-P005-2017) Optimizing the Flux Pinning of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ Superconductor with BaHfO_3 and Y_2O_3 Mixed Phase Additions

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Adding nanophase defects to $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) superconductor thin films is well-known to enhance flux pinning; resulting in an increase in current density (J_c). While many previous studies focused on single phase additions, the addition of several phases simultaneously shows promise in improving current density by combining different pinning mechanisms. This paper studies the effect of the addition of insulating, nonreactive phases of barium hafnate (BHO) and yttrium oxide (Y_2O_3) to YBCO thin films. Processing parameters varied the target composition volume percent of BHO from 2 – 6 vol. %, while maintaining 3 vol. % Y_2O_3 , and the remaining vol. % YBCO. Pulsed laser deposition produced thin films on LaAlO_3 (LAO) and SrTiO_3 (STO) substrates at various deposition temperatures. Comparison of strong and weak flux pinning mechanisms, current densities, critical temperatures, and microstructures of the resulting films will be presented.

(EMA-P006-2017) A Facile Method to Synthesize Highly Conductive Polymer Derived Ceramics with Arbitrary Shapes by Built-in Conductive Networks

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In this paper, we proposed a prototype of synthesizing conductive polymer derived ceramics (PDCs) by using the built-in conductive networks. The conductive networks were formed by attaching the edge functionalized graphene oxide (EFGO) to the commercial polyvinyl alcohol (PVA) foams. After immersing the homemade conductive networks into the precursor of polysiloxanes, the composites were cured and pyrolyzed to form networks embedded conductive PDCs. Desired shapes of the PDCs are convenient to be realized because the PVA foams are quite soft to be cut. The conductivity of the networks embedded PDCs can be up to 0.94 S/cm at room temperature, and the conductivity of that PDC at the environmental temperature of 600 Celsius was increased to 1.7 S/cm. The huge electrical conductivity improvement of PDCs after pyrolysis compared to the precursor of polysiloxanes was contributed to the built-in conductive networks and the graphitic domains formed within the matrix during the pyrolysis.

(EMA-P007-2017) Study of the local structures of $\text{Bi}(\text{Zn}_{2/3}\text{Nb}_{1/3})\text{O}_3$ -based systems

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Perovskite solid solutions containing $\text{Bi}(\text{Zn}_{2/3}\text{Nb}_{1/3})\text{O}_3$ (BZN) show useful dielectric properties. Using diffraction, it was previously reported that in $(1-x)\text{PbTiO}_3$ - $x\text{Bi}(\text{Zn}_{2/3}\text{Nb}_{1/3})\text{O}_3$ (PT-xBZN), increasing the BZN content ($x < 0.3$) increases the tetragonality and Curie temperature. However, alloying with BaTiO_3 (BT-xBZN) led to a lower tetragonality than BT ($x < 0.125$), and this system exhibited relaxor behaviors when $x > 0.062$. Consideration of the local structure in these systems is an important aspect for developing structure-property relationships and was therefore undertaken in this work. In our study, synchrotron X-ray total scattering was conducted on 6 samples of different compositions, (BT-xBZN ($x=0.025, 0.05$ and 0.1) and PT-xBZN ($x=0.05, 0.2$ and 0.3)). Their

pair distribution functions (PDFs) were obtained from the scattering data. Box-car fitting was performed on the PDFs to obtain the length-scale dependent lattice parameters. The results show the tetragonality of the local structure is enhanced compared to the average structure for all BT-xBZN samples. With increasing BZN content, the tetragonality of the average structures decreases, while the local-scale distortion actually increases. In contrast, there is no local distortion enhancement in PT-xBZN. With the PDF analysis, we can explain how composition affects the local structure, and further enhance structure-property relationships.

(EMA-P008-2017) Structure-property relationship of the piezoelectric system $x\text{BiInO}_3-(1-x)\text{BaTiO}_3$

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The purpose of this study is to investigate the structure-property relationship of the system $x\text{BiInO}_3-(1-x)\text{BaTiO}_3$ in the region $0.03 \leq x \leq 0.12$. Here, we study the physical properties and the structure of the solid solution between the Bismuth-based material BiInO_3 (BI) with orthorhombic space group $\text{Pna}2_1$, and the classical piezoelectric material BaTiO_3 (BT) with tetragonal structure, $\text{P}4\text{mm}$, and $d_{33} = 190 \text{ pC/N}$. Based on a structural analysis work previously carried out by Datta et al., they claimed that there is a morphotropic phase boundary (MPB) for the system $x\text{BiInO}_3-(1-x)\text{BaTiO}_3$ at $x = 0.1$ where two phases coexist ($\text{P}4\text{mm}$ and $\text{R}3\text{m}$). In this study, we have found that there is actually an MPB where the electromechanical properties are maximized but at $x = 0.065$. The effective piezoelectric coefficient values for $x = 0.03, 0.065$ and 0.12 are 120, 260 and 25 pm/V respectively and the maximum polarization values obtained from the polarization versus electric field loops for $x = 0.03, 0.065$ and 0.12 are 9.9, 12.6 and 5.9 $\mu\text{C/cm}^2$ respectively. In conclusion, we have proved that for the system $x\text{BiInO}_3-(1-x)\text{BaTiO}_3$ an MPB exists where the electromechanical properties are maximized at $x = 0.065$ and the structure has been reinvestigated.

(EMA-P009-2017) Nanostructured $\text{Al}^{3+}/\text{Mn}^{2+}$ doped ZnO ambigels as electrodes for supercapacitors

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Efforts have been made to satisfy the requirements of electrochemical energy storage, such as supercapacitors, through the use of low cost and environmentally friendly materials combined with ease of fabrication. Transitions metal oxides are promising materials for supercapacitors due to their excellent pseudocapacitive properties and their fast and reversible redox reactions. ZnO xerogels and ambigels incorporated with Al e Mn were in situ produced by sol-gel synthesis, followed by controlled drying. A device consisting of a PVA/ H_3PO_4 membrane (separator/electrolyte) uniformly coated with 0.5 mg of the electrode powder on each face and copper foils as metallic contact was mounted and electrochemically characterized. ZnO xerogels presented specific capacitance of 19 F.g^{-1} , while ZnO ambigel presented a capacitance of 86 F.g^{-1} . The ambigel of ZnO/2%Al presented a specific capacitance of 375 F.g^{-1} and the ambigel of ZnO/2%Mn exhibited a specific capacitance of 590 F.g^{-1} . Both ambigels of ZnO incorporated with Al and Mn presented values of energy density and power density that classify them as supercapacitors. The ZnO/2%Mn ambigel delivered a maximum energy density of 0.8 Wh.kg^{-1} and a maximum power density of 47 kW.kg^{-1} . The results indicate the potential of nanostructured ZnO doped with Al or Mn as electrodes for supercapacitors.

(EMA-P010-2017) Pathways of Polarization Reversal

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Polarization in ferroelectric materials is induced through several mechanisms (e.g. polarization switching, ionic and atomic polarization). Polarization switching can occur through the motion of planar defects such as domain walls. In ferroelectric materials, two forms domain wall motion are present, i.e. non-180° and 180° (domain reversal). Recent time-resolved in situ X-ray diffraction experiments have suggested that domain reversal can be achieved through multiple non-180° reorientation events. In this paper, we present a time-resolved in situ X-ray diffraction study that investigates the polarization reversal mechanisms in the $(1-x)\text{BaTiO}_3-x\text{BiZn}_{0.5}\text{Ti}_{0.5}\text{O}_3$ (BT-BZT) system. Time resolved diffraction data from BT, 0.94BT-0.06BZT, and 0.92BT-0.08BZT was measured with 10 ms time resolution. We show that polarization reversal in BT is achieved through direct inversion of spontaneous dipoles. However, the addition of BZT into BT promotes a two-step polarization reversal process (i.e., two consecutive non-180° reorientation events). The intermediate (non-180°) polarization state in 0.94BT-0.06BZT is accommodated by a lattice expansion perpendicular to the field. The results will be discussed in the context of other Pb-, Bi-, and Ba-based compositions, including relaxor-like compositions.

(EMA-P011-2017) Phase stability and B-site ordering in $\text{La}_2\text{NiMnO}_6$ thin films

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With its high paramagnetic-to-ferromagnetic Curie temperature (~280 K) and good magnetic properties near room temperature, the multiferroic (ferroelectric and ferromagnetic) double-perovskite $\text{La}_2\text{NiMnO}_6$ has been considered as a promising candidate of ferromagnetic semiconductor for magnetoelectronics and spintronics, and thus attracted much research attention in recent decades. The microstructure and physical properties of $\text{La}_2\text{NiMnO}_6$ in the form of thin films can be influenced by many factors, e.g. the growth conditions including growth temperature and oxygen pressure, and the epitaxial strain induced by the film-substrate lattice mismatch. In this work, thin films of multiferroic double-perovskite $\text{La}_2\text{NiMnO}_6$ are prepared on (001)-oriented SrTiO_3 , $(\text{La}_{0.289}\text{Sr}_{0.712})(\text{Al}_{0.633}\text{Ta}_{0.356})\text{O}_3$ and LaSrAlO_4 substrates by pulsed laser deposition. Microstructure investigation by advanced electron microscopy shows that the $\text{La}_2\text{NiMnO}_6$ films have a monoclinic structure on the SrTiO_3 substrates and a rhombohedral structure on the $(\text{La}_{0.289}\text{Sr}_{0.712})(\text{Al}_{0.633}\text{Ta}_{0.356})\text{O}_3$ and LaSrAlO_4 substrates. Atomic-scale elemental maps of the monoclinic and rhombohedral phases reveal a short-range and/or partial ordering of the B-sites. In addition, domains and columnar grains are found in the films. Our results demonstrate that the phase and microstructure of the $\text{La}_2\text{NiMnO}_6$ films can be tuned by epitaxial strains induced by different substrates.

(EMA-P012-2017) Dielectric relaxation and Impedance spectroscopic studies of $(\text{Li}/\text{Ta}/\text{Sb}) (\text{Na},\text{K})\text{NbO}_3$ ceramics with excess Na

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NaNbO_3 (NKN) system exhibits the highest performance in practical device applications because of the morphotropic phase boundary usage. Alkaline niobate based system NKN which is a solid solution of anti-ferroelectric NaNbO_3 and ferroelectric KNbO_3 is one of the prominent member of the lead free family with properties comparable to PZT systems and wide operating temperature ranges.

In this study, lead-free ferroelectric ceramics ($\text{Li}_{0.04}(\text{Na}_{0.54+x}\text{K}_{0.46})_{0.96}(\text{Nb}_{0.81}\text{Ta}_{0.15}\text{Sb}_{0.04})\text{O}_3$ with $x=0.00, 0.005$ and 0.01) were synthesized by solid state sintering technique. X-ray diffraction analysis of the samples showed an orthorhombic structure with a secondary phase which decreased with increasing Na content. A high remnant polarization and low leakage current was observed for $x=0.01$ composition. With increase in Na content, Curie temperature (T_c) shifted to higher temperature side and the ferroelectric and dielectric properties were improved. Addition of excess Na at A-site helps in suppressing the volatility and maintains the stoichiometry and composition of the sample. Impedance spectroscopic measurement showed that the value of real part of impedance decreased with rise in temperature and exhibited negative temperature coefficient of resistance (NTCR) behavior. Imaginary part of impedance suggested the presence of weak dielectric relaxation above 300°C in these ceramics.

(EMA-P013-2017) Electrical and dielectric behaviour of microwave sintered (K,Na,Li)NbO₃ Lead free ceramics

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Recent concern over the environment requires the development of lead-free piezoelectric materials. Due to its high dielectric and piezoelectric properties, potassium sodium niobate, (K,Na)NbO₃, and related materials have been considered as one of the promising candidates for lead-free piezoelectric materials. The conventional solid state synthesis method usually needs relatively high calcination temperatures and sintering temperatures at which the evaporation of Na₂O and K₂O could become more serious. Therefore, if a high piezoelectric performance of (K,Na)NbO₃ ceramics is to be obtained, a more effective powder synthesis method and sintering process, which reduces the volatilization of alkaline elements, should be developed. In this work, lead-free piezoelectric ceramics of Li substituted (K_{0.5}Na_{0.5})NbO₃ (KNN) were produced by microwave sintering to reduce the volatilization of the alkaline elements. X-ray diffraction (XRD) studies at room temperature confirmed the formation of orthorhombic perovskite structure. Scanning Electron Micrographs suggest polycrystalline microstructure with grains of unequal size distributed throughout the samples. Complex impedance spectroscopy analysis indicated negative temperature coefficient of resistance behavior, identical to semiconductors.

(EMA-P014-2017) High-Pressure Synthesis of A-Site Ordered Double Perovskite CaMnTi₂O₆ and the Origin of its Ferroelectricity

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Recently, we synthesized LiNbO₃-type MnBO₃ (B = Ti, Sn) and discovered magnetoelectric coupling for these compounds. However, these compounds did not exhibit ferroelectricity due to their leakage current and high coercive field. Therefore, MnTiO₃-CaTiO₃ solid solution has been studied to improve the dielectric properties for MnTiO₃. As a result, we found the novel polar A-site ordered perovskite CaMnTi₂O₆. In this study, we investigated structural and dielectric properties of CaMnTi₂O₆ and elucidated the origin of ferroelectricity. CaMnTi₂O₆ reacted at 7 GPa and 1200°C crystallizes in a tetragonal A-site ordered perovskite-type structure with a polar space group P₄mc. The structure is characterized by the columnar ordering of Ca²⁺ and Mn²⁺ ions along c axis and Mn²⁺ has tetrahedral and square-planar geometry. Polarization reversal was observed by the P-E hysteresis loop measurement. Probably, the weak binding for Mn²⁺ suggested by long Mn-O bond length results in easy polarization reversal. Temperature dependences of dielectric permittivity, second harmonic generation, differential scanning calorimetry, and synchrotron X-ray diffraction measurements showed that CaMnTi₂O₆ underwent ferroelectric phase transition around 630 K. The structural change across phase transition suggested that

in CaMnTi₂O₆, cooperative shifts of Mn²⁺ and Ti⁴⁺ result in ferroelectric distortion.

(EMA-P015-2017) Neutron Diffraction and Magnetic Studies on PbFe_{0.5}Nb_{0.5}O₃-BiFeO₃ Solid Solutions

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PbFe_{0.5}Nb_{0.5}O₃ is a well-known multiferroic exhibiting magnetoelectric coupling below its Neel temperature (T_N) – 155 K and it has ferroelectric $T_C = 385$ K. BiFeO₃ is the only room temperature magnetoelectric multiferroic and its T_N is 643 K and T_C is 1103 K. We made an attempt to synthesize single phase (1-x) PbFe_{0.5}Nb_{0.5}O₃ - (x) BiFeO₃ solid solutions with $x = 0.1, 0.2, 0.3$ and 0.4 by single step solid state reaction method. Structural studies have been carried out through XRD and it reveals the formation of single phase and also we observed the structural phase transition from monoclinic (Cm) to rhombohedral (R3c) at $x = 0.4$. In order to understand the nuclear and magnetic structure, room temperature neutron diffraction studies were carried out for all the solid solutions. Neutron Diffraction studies reveals the origin of magnetic ordering at RT from $x = 0.2$ onwards and it confirms the G type antiferromagnetic ordering. Room temperature Electron Paramagnetic Resonance showed the paramagnetic nature for $x = 0.1$ and 0.2 whereas for $x = 0.3$ and 0.4 it shows the antiferromagnetic origin. Temperature dependent magnetic susceptibility shows the tuning of T_N from 230K to 350K for $x = 0.1$ to 0.4 . Temperature dependent dielectric studies show the evidence of existing magnetoelectric coupling.

(EMA-P016-2017) Measuring Energy Density and Dielectric Breakdown in Polymers and Polymer Ceramic Composites

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In the literature there are many ways that researchers have measured or calculated the energy density and dielectric breakdown of polymer films and polymer ceramic composites. Due to the fact that no standardized units or techniques have been officially agreed upon, it is very difficult to compare and understand results across research groups. Several years ago, under the ONR Capacitor program, we led a tri-service effort to create procedures accurately measure properties for pulse power applications. This poster will demonstrate the differences between the standard measurements on ceramics compared to polymer films. In addition, we will cover the pitfalls and problems with these measurements.

(EMA-P017-2017) Growth and Properties of Tin Oxynitride Thin Films

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Oxynitride, where both oxygen and nitrogen ions are bonded with metal cations, is gaining more attention for its potential benefits of merging physical properties of oxides and nitrides. Controlling oxygen/nitrogen ratio can provide a tool to engineer the bandgap, the electrical conductivity, and the crystal structure. Moreover, the different ionicity/covalency of oxygen and nitrogen may play a unique role to determine the physical properties of oxynitrides. Here, recent results will be reviewed on the epitaxial growth of tin oxynitride thin films using reactive sputtering technique and the characterization of their physical properties. Our results will provide new opportunities to design novel properties of materials for next-generation electronics as well as to explore physics on aliovalent anion substitution.

(EMA-P018-2017) Towards the rapid synthesis of high-quality monolayer continuous film of graphene on the plasma modified Cu foil with high surface free energy

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Graphene and chemical vapor deposition (CVD) technique provide large area extraordinary 2D material with the unique feature of transferability to modern electronics. Here, we are reporting the use of high surface free energy (SFE) and nano-scale high-density surface kinks existing Cu foil for CVD graphene growth, which is an opposite approach to modern use of catalytic surfaces for high-quality graphene growth. But, we observed controllable rough morphological nature opens a new era for fast synthesis of graphene as a continuous film while maintaining a high monolayer ratio. High energy Ar plasma treatment on Cu surface, makes it rougher and high SFE condition and further, introduced kink-like area on Cu(100) crystal plane facilitated to faster nucleation with a high monolayer ratio (I_{2D}/I_G is 2.42). The fast nucleation and growth avoid the diffusion of C atoms to Cu-graphene interface, which is resulting in the negligible formation of bilayer patches. Even though, it fails to maintain defect-free condition (I_D/I_G is 0.46) due to high SFE. However, a short H_2 gas post-annealing step which followed by graphene growth facilitated improving quality of the graphene. In this presentation, a detailed overview of modification Cu surface, and its effect on the nature of graphene and quality enhancement due to post-treatment will be presented.

(EMA-P019-2017) Fabrication of transparent electrode for near UV range applications by using ITO nano dots/ ITO thin film by organic additives-free sol-gel technique

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Indium tin oxide (ITO) still remains the industrial standard transparent conducting oxides with better performances. 10 wt.% tin-doped, ITO nano dots and thin film were prepared by an environmentally friendly aqueous spin coating technique with $In(NO_3)_3 \cdot H_2O$ and $SnCl_4$ without using organic additives. The wettability and surface free energy (97.6986 mJ/m²) enhanced oxygen plasma treated glass substrates were used to form an ultra thin voids free continuous ITO film. The spin-coated samples were annealed at above 400°C for 1 hour under low vacuum conditions to obtained crystallized, thin ITO film. X-ray diffraction patterns reveal that the films contain the In_2O_3 phase only and exhibit the polycrystalline nature of the cubic structure with the main peak of (222) plane. Further, annealing at the higher temperature (600°C) improved the degree of crystallinity which facilitated increment of the band gap, enhanced transmittance (86.43 % at 550 nm) and electrical characteristics ($1.68 \times 10^{-3} \Omega cm$). The peak positions of $In 3d_{5/2}$ (444.28eV) and $Sn 3d_{5/2}$ (486.7eV) in XPS results indicated that indium and tin are in the oxide form only. In the presentation, the effect of oxygen plasma treatment on quality of the thin film, the characteristics of ITO film and the ITO nano dots to enhance the performances of graphene will be addressed.

(EMA-P020-2017) Complex Site Occupancy and Mesoscale Chemical Heterogeneity of $(1-x)BaTiO_3 - xBi(M)O_3$ Dielectrics

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The purpose of this study was to map out correlations among dielectric properties, microstructure, and cation size of a selection of $(1-x)BaTiO_3 - xBi(M)O_3$ ceramic compositions (where M denotes a net-trivalent cation or cation pair occupying the B-site of the perovskite structure) in an effort to better understand their behavior. The compositions studied were $(1-x)BaTiO_3 - xBi(Zn_{1/2}Ti_{1/2})$ ($x=0.10, 0.20$), $(1-x)BaTiO_3 - xBi(Zn_{2/3}Nb_{1/3})$ ($x=0.065, 0.10$), $(1-x)BaTiO_3 - xBi(Mg_{1/2}Ti_{1/2})$ ($x=0.06, 0.10$), and $(1-x)BaTiO_3 - xBi(Mg_{3/4}W_{1/4})$ ($x=0.07, 0.15$); each of these shows promise as a dielectric in capacitors that are capable of operating at elevated temperatures and under

large applied electric fields. Rietveld refinements of high-resolution synchrotron powder diffraction data (collected at Beamline 11-BM at the Advanced Photon Source at Argonne National Laboratory) enabled direct comparison of the effect of different cations on variable site occupancy and subtle structural variations of the unit cell. In some cases the refinements were able to distinguish structurally similar but chemically distinct perovskite phases that were not detectable using typical laboratory x-ray diffraction techniques. Correlating these data with the measured dielectric properties of each composition provided insights to the underlying mechanism and defect chemistry responsible for the performance of these materials.

(EMA-P021-2017) Prediction of 2D transition metal trihalides

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Density-functional theory calculations of layered 3d shell transition metal halides (MX_3) predicts that these materials can exist nearly degenerately in a variety of crystal structures with interesting magnetic and electronic properties. The most often space groups encountered are $R\bar{3}$, $P3_112$ and $C2/m$. Based on reaction enthalpies calculated between the MX_3 compounds and their most stable competing phases, 16 compounds are predicted to be thermodynamically unstable by less than 200 meV/atom, indicating they may exist as a metastable structures during experimental synthesis of monolayers, which means that they are likely be able to get synthesized into 2D materials by exfoliation method. FeX_3 and CrX_3 ($X = Cl, Br$ or I), along with VCl_3 and $RuCl_3$, are shown to have very strongly magnetic ground states. For some of the compounds, we found that magnetic moment changes greatly when we compare bulk to the layered structure. We discuss the electronic structure and magnetic anisotropy of these novel 2D materials and their potential for spintronic applications.

(EMA-P022-2017) Technique development for studying origins of microcracking due to inhomogeneous stresses

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Electric-field-induced microcracking is common in piezoelectric materials due to their electromechanical response. It is known that, at low electric field values, the formation and propagation of microcracks is the dominant mechanism of electrical fatigue, and macrocracks are generated at high electric field amplitudes. In multilayer ceramic actuators (MLCAs) and capacitors (MLCCs), stresses can be largely inhomogeneous near electrode edges, exacerbating cracking and fatigue. However, few details are known about the parameters controlling microcracking in multilayer stacks, where inhomogeneous stresses appear between electrically active and inactive regions. In order to simulate the inhomogeneous stresses, finite element modeling of multilayer stacks was performed in ANSYS. The models predict that the stress at the electrode tips and dead zones is higher than between the electrodes. Experimental techniques are also being developed to characterize the spatial distribution of microcracks and, specifically, their relationship to stress concentrations and gradients and grain misorientations. Initial experimental results obtained from electron backscatter diffraction (EBSD) and Transmission Kikuchi Diffraction (TKD) will be presented. The results contribute to a fundamental knowledge of cracking and fatigue in piezoelectrics and will help in the design of new actuator and capacitor components.

(EMA-P023-2017) Electrolytic Deposition of Copper from Ammonia-Ammonium Sulfate Solution Containing Cu(I)

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A large amount of copper is used in various electric appliances, cable, motor vehicles and so on. However, the reserve/production ratio for copper is only 30 years. Therefore, the copper recovery from

the waste materials is indispensable. Therefore we have investigated copper electroplating from ammonia-ammonium sulfate solution containing Cu(I) in order to develop an energy-saving hydrometallurgical process. In the present study, the influence of electrolytic conditions on the morphology of the deposits has been examined. The cathodic solution was prepared from cuprous oxide (Cu_2O), NH_3 solution and $(\text{NH}_4)_2\text{SO}_4$. The working electrode was a copper plate. The counter electrode was a platinum plate. The reference electrode was an AgCl-Ag electrode. All experiments were performed under an argon atmosphere at room temperature. Potentiostatic electrolysis was conducted on the copper electrode in $5.0 \text{ kmol m}^{-3} \text{ NH}_3$ and $1.0 \text{ kmol m}^{-3} (\text{NH}_4)_2\text{SO}_4$ containing $0.50 \text{ kmol m}^{-3} \text{ Cu(I)}$. A smooth plate, a crowd of whiskers and a crowd of nodules were obtained at -0.30 , -0.50 and -0.80 V , respectively, by 20 h electrolysis. Galvanostatic electrolysis was also conducted on the copper electrode for 20 h . The copper deposit was smooth at (a) 300 A m^{-2} , while a crowd of nodules was obtained at (b) 700 A m^{-2} . The current efficiencies of copper electrodeposition were 92% or higher at all conditions.

(EMA-P024-2017) Mass Production of High Quality Boron-doped Diamond Thin film by Surface Wave Plasma CVD

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Boron doped diamond (BDD) film is excellent electrode material as an anode for waste water treatments system because of its excellent mechanical properties, wide potential window, low background currents and electrochemical stability. In the industrial mass production, it is highly desirable to develop a large area (or large scale) BDD film through the low temperature synthesis. Generally, BDD electrode reported in many researches was synthesized by micro wave plasma chemical vapor deposition (MPCVD). However, it is impossible to use for the industrial mass production of BDD films due to the high process temperature and small deposition area ($<50 \text{ mm}$ diameter). In this study, we have successfully designed micro wave plasma chemical vapor deposition (MPCVD) system into surface wave plasma (SWPCVD) system to synthesize BDD films on Si wafer ($\text{Ø}150 \text{ mm}$) with various working pressure from 260 to 815 mtorr

(EMA-P025-2017) Development of radiotransparent ceramic based on composition of the system $\text{BaO-SrO-Al}_2\text{O}_3\text{-SiO}_2$

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The work represents results of investigation that directed to development of compositions and technological parameters for obtaining radiotransparent ceramic and investigation of their properties in relation to structure and phase composition. As a basis for obtaining a ternary system $\text{BaO-SrO-Al}_2\text{O}_3\text{-SiO}_2$ was chosen. Considering phase properties in this system, for synthesis of ceramic with low coefficient of radiowave diffraction and high heat resistance slawsonite and celsian phases were chosen. For investigation of possibility to create radiotransparent materials three oxide compositions were chosen. Ratio of $\text{SrAl}_2\text{Si}_2\text{O}_8\text{:BaAl}_2\text{Si}_2\text{O}_8$ phases were changed as: C1 – 1:3; C2 – 1:1 and C3 – 3:1. For increasing of sintering degree as a mineralizer $2 \text{ wt.}\%$ of Li_2O (over 100% dry substance). In the result of carried experimental researches, materials of celsian-slawsonite composition were obtained that characterized by high density, mechanical strength and satisfy the requirements that set up to electro-physical characteristics of radiotransparent materials. Investigation results allow to set an optimal composition and sintering conditions, which allow to obtain materials with low amount of additional phases and complex of optimal properties: $W = 0,07 \div 0,25\%$, $\rho_{\text{app}} = 2960 \div 3025 \text{ kg/m}^3$; $\varepsilon = 7,3 \div 8,7$; $\text{tg}\delta = 0,0077 \div 0,0096$; $\sigma_{\text{com}} = 109,14 \div 182,95 \text{ MPa}$; $\sigma_{\text{flex}} = 15,82 \div 34,66 \text{ MPa}$.

(EMA-P026-2017) Crystalline tellurite optical fiber development for hydrophone

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Tellurite-based materials have generally few compromising properties between oxide (i.e. silica, silicate, etc.), fluoride and chalcogenide materials in terms of IR transmission ranges, nonlinearity and processing. Although chalcogenide has higher refractive index and longer IR transmission in comparison to tellurite material, it suffers from extreme processing difficulty, higher loss in visible spectra, low damage threshold, and multiphoton absorption. Furthermore, tellurite has very high sensitivity of acousto-optics (AO) effect. In this study, we first fabricate polycrystalline tellurite in amorphous matrix and then (poly)crystalline tellurites and their optical fibers for hydrophone. Although tellurite in amorphous is expected to have lower acousto-optics effect, they are much easy to processing into various forms and may promote novel applications such as coupler and others. Furthermore, improving the AO effect of polycrystalline tellurite in amorphous matrix by processing is one of main goal in this study. Both single-mode and multimode tellurite optical fiber are to be made. Compared with conventional piezoelectric hydrophone, their AO dependence on acoustic frequency (10 Hz to 5.6 MHz or more), acoustic intensity (70 to -236 dB), and directional sensitivity to the incident direction of an acoustic will be presented and their potential applications will be discussed.

(EMA-P027-2017) Study on Field Assisted Sintering of CaLa_2S_4 Powders Processed via High-Energy Ball Milling

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The Field Assisted Sintering Technique (FAST) has been widely researched and applied in the consolidation of various oxide and non-oxide ceramics. In this study, FAST was used to consolidate calcium lanthanum sulfide (CaLa_2S_4) ceramics for infrared optical ceramics applications, with broader infrared transmittance and higher rain erosion resistance. High-energy ball milling was applied to process commercially sourced CaLa_2S_4 powders, in order to investigate the influence of particle size and morphology on the sintering activity of the powders. The sintering behavior and grain growth kinetics of the CaLa_2S_4 ceramics during the FAST process were studied through shrinkage curve measurements and microstructural characterization. Mechanical properties measurements were performed to determine the relationships between the grain size, density, and hardness of the CaLa_2S_4 ceramics. Spectroscopic characterization included measurements and analyses of infrared transmittance and photoluminescence behavior. The electrical properties of the CaLa_2S_4 ceramics were also characterized in order to gain insight into the defects present in the as-sintered ceramics.

(EMA-P028-2017) Study of solid-state conversion of non-oxide crystals

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In order to investigate the effects of various processing parameters on the solid-state conversion of ceramics into single crystals, the properties of two fluoride materials (CaF_2 and $\text{Sr}_3(\text{PO}_4)_3\text{F}$) treated under different sintering and annealing conditions were examined. A conventional pressureless thermal treatment was first performed to sandwich a single crystalline and polycrystalline specimen together, during which crystal growth was minimal. Spark plasma sintering and a modified pressureless spark plasma sintering process were subsequently employed to further study the effect of electric field and pressure on crystal growth. Results show that the presence of an electric field and the Joule heating it produces is critical in achieving effective densification and the retardation of grain growth, which is essential in controlling grain energy and promoting the seed crystal growth. In addition, a similar degree of crystal growth was observed in ceramics with different structures and grain morphologies, indicating that grain structure has only a weak influence on the migration of the single crystal boundary. This parametric study may

act as inspiration for a deeper exploration of the field of solid-state conversion.

(EMA-P029-2017) Nanostructured ZnO/Graphene xerogels with photosensing properties

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Graphene based nanocomposites with emerging optoelectronic properties have been developed for applications as photodiodes and solar cells. In this work ZnO/graphene nanocomposites were produced in situ with different graphene concentrations through the sol-gel method. Drying in air for 24 h led to a bulk xerogel structure. Electrical characterization was performed by tracing the I-V curves of the nanocomposites in the dark and under different illumination conditions (visible and UV light). Significant current variation, from 10 nA to 10 μ A, was observed for the different graphene containing samples depending on the wavelength and light intensity. Moreover the photocurrent increased with graphene content for the same lightning condition. The highest photosensitivity was recorded for the nanocomposite with 5 wt.% graphene. The results indicate the potential of the developed ZnO/Graphene nanocomposite in applications like photodiodes, photoresistors and solar cells.

(EMA-P030-2017) Rare-earth ions doped heavy metal borate scintillators

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Recently, great importance has been devoted to different glass systems doped with rare-earth ions because of their peculiar properties, in particular in the field of high-energy physics for particle energy measurement. Borate glass has been found to be a suitable optical material, on the other hand heavy metal component in glass matrix enhance scintillating properties for rare-earth ions. The purpose of the present study was to investigate the optical and physical properties of Dy³⁺, Er³⁺, Nd³⁺, Ce⁴⁺ doped heavy metal glasses, with various rare-earths oxide concentrations, in order to satisfy the requirements necessary for particle energy measurement. High density, low refractive index, high emission intensity and high lifetime decay are required for this purpose. The structural properties has been measured through X-ray diffraction and Raman spectroscopy in order to evaluate the amount and type of crystalline phases inside the glassy structure. The physical properties have been related with the structural properties. All the investigated glasses have shown peculiar characteristics that if properly tuned can match the requirements needed for particle energy measurement. Crystalline phases promotes scintillating properties as intensity and lifetime decay. In this study has been demonstrated that crystalline phases are enhanced mainly in the glasses containing Al₂O₃ above 1mol% and Ce⁴⁺ as scintillating dopant.

(EMA-P031-2017) The photo-detecting transistor based on graphene/BiFeO₃ heterostructure

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Graphene have rapidly developed as intriguing building blocks for electronic, energy and optoelectronic application. However, due to the absence of semiconducting gap, charge carrier modulation in graphene through electrostatic doping is required. Here, we demonstrated photo-detecting transistor based on graphene channel on BiFeO₃ thin film and nano island. Ferroelectric polarization can drive spatially local manipulation of carrier density and type in the graphene via electrostatic doping. This transistor exhibited various resistance states originating from the coupling of semiconducting behavior of graphene channel and the polarization of BiFeO₃. Furthermore, the creation of spatially defined p-n junctions in

graphene by local polarization switching is of critical importance for the tunable optical properties and transport properties. Our study could provide a new route for developing advanced nanoelectronic and optoelectronic devices.

(EMA-P032-2017) DFT Prediction and Characterization of Two-Dimensional Group-III Chalcogenides

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The remarkable properties of graphene and layered MoS₂ have piqued the interest in two-dimensional materials with unique electronic and optical properties. By performing chemical substitutions in the single layer Al₂O₃, B₂O₃ and Sb₂O₃ structures using elements from the group-III and chalcogen family, we identify a novel group of two-dimensional M₂X₃ compounds. Using density-functional theory calculations, we determine the formation energies of these 2D compounds. These structures are then characterized through using PBE and hybrid exchange-correlation functionals for their electronic and optical properties. We found several compounds that can be grown using CVD or MBE and have metallic and semiconducting characteristics.

(EMA-P033-2017) Synthesis of Magnetoelectric Composites on a Single Nanoparticle

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Magnetoelectric composites present a unique opportunity to be able to control the magnetization of a material using electric fields, and similarly, to control the polarization of a material using magnetic fields via the magnetoelectric effect. However, these have traditionally been fabricated in bulk form. Here, we present work on the synthesis of bi-phasic magnetoelectric Janus nanoparticles composed of piezoelectric barium titanate and magnetostrictive cobalt ferrite via sol-gel electrospraying. In these composite magnetoelectrics, the interface between the phases is important for the strain transfer that results in the magnetoelectric effect. It is predicted that the increased ratio of interfacial area to volume in magnetoelectric nanoparticles will result in an enhanced magnetoelectric effect. Particle morphology was examined using both scanning electron microscopy and transmission electron microscopy. X-ray diffraction was used to confirm the presence of tetragonal barium titanate and spinel cobalt ferrite as well as to determine the weight ratio of barium titanate to cobalt ferrite. SQUID magnetometry was used to confirm particle composition by comparing the saturation magnetizations of cobalt ferrite particles and Janus particles. In addition, vibrating sample magnetometry was used to qualitatively examine the magnetoelectric nature of the particles.

(EMA-P034-2017) Van der Waals Epitaxy of Layered Halide Perovskites

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Organometal halide perovskites and layered materials have both emerged as promising candidates for the exploration of new physics and high performance optoelectronic devices. Under this circumstance, layered organometal halide perovskites, with the merit of both, have been studied extensively for their naturally quantum well structures and high exciton binding energy. In this report, we demonstrate the epitaxial growth of layered perovskite (C₄H₉NH₃)₂PbI₄ on muscovite mica by vapor phase epitaxy. With elaborated growth process, square-shaped single crystalline films with few-layer thickness and high surface smoothness were synthesized. Owing to van der Waals epitaxial growth, the orthorhombic (C₄H₉NH₃)₂PbI₄ films were aligned with c axis perpendicular to mica surface and a/b axis conformed to the hexagonal symmetry of substrate. Excitonic emission of (C₄H₉NH₃)₂PbI₄ was also studied by temperature dependent photoluminescence. Our study may shed new light on the role of van der Waals interactions in low dimensional thin film growth and provide new solutions to vapor phase epitaxy of soft layered materials.

(EMA-P035-2017) Thermal stability and brazing of thermoelectric tellurides

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One of the biggest obstacles in generating a working thermoelectric generator is turning materials into functional devices. Challenges that must be overcome include thermal stability at the material level and reliable contacts at the device level. In this research we extend from basic materials research, toward testing and improving some of the challenges to broad applications. For approaching practical thermoelectric power generation devices, highly reliable telluride materials were implemented. Thermal cycling tests were conducted in order to evaluate their thermal stability in long term usage. Brazing compositions based on Mn-Sn and Ag-Cu-In were considered for bonding of thermoelectric material into Co and Fe bridges. The final goal of the research is achieving a generator prototype which will work in a lab testing facility.

(EMA-P036-2017) Effect of Pb doping on thermoelectric properties of $\text{Bi}_{1-x}\text{Pb}_x\text{CuOSe}_{0.8}\text{Te}_{0.2}$

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Thermoelectric materials have received much attention as one of the alternative energies of fossil fuel. BiCuOCh ($\text{Ch} = \text{Se}$ and Te) oxychalcogenides are one of promising thermoelectric materials which can be used at mid-high temperature due to their intrinsically high Seebeck coefficient and low thermal conductivity. The improved efficiency of BiCuOCh has been achieved through doping, formation of vacancy, or texturing. However, only Sr doping effects on thermoelectric properties of $\text{BiCuOSe}_{1-x}\text{Te}_x$ at room temperature were reported. In this work, the effect of Pb doping on the thermoelectric properties of $\text{Bi}_{1-x}\text{Pb}_x\text{CuOSe}_{0.8}\text{Te}_{0.2}$ compounds ($x = 0 \sim 0.6$) were investigated. With increasing amounts of Pb doping, the hole concentration was increased, resulting in the increase in the electrical conductivity and the decrease in Seebeck coefficient. The highest ZT was obtained in $\text{Pb}_{0.06}\text{Bi}_{0.99}\text{CuOSe}_{0.8}\text{Te}_{0.2}$ compound at 911K with optimized hole concentration in spite of the increase in total thermal conductivity caused by the electronic contribution.

(EMA-P037-2017) High-Thermoelectric Performance of Metal-oxide Coated Bismuth Antimony Telluride Alloys

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Recently, thermoelectric materials combined with nanotechnology have shown possibility of greatly improving thermoelectric performance based on nanometer-scale phenomena such as electric filtering and phonon scattering. For practical uses of thermoelectric materials, it is considered that figure of merit (ZT) of 2 or above should be met, although the reported ZT has been obtained to 1 near room temperature. In this study, we develop a novel bismuth antimony telluride (BST) alloy made of BST powders coated with nanometer-scale metal-oxide (ZnO) layer using conventional atomic layer deposition technique. In order to evaluate the effect of such core-shell type materials, we measure ZT of the ZnO / BST alloys over a temperature range of 300-500 K. The ZnO layer serves to reduce thermal conductivity without the decrease of electrical conductivity, leading to the enhancement of ZT. Thin ZnO layer is believed to scatter short-wavelength phonons while enables the electrical transport without the loss of electrical conductivity. The detailed thermal and electrical properties of the ZnO coated BST alloys will be discussed in terms of ZnO / BST core-shell structure and energy band filtering effects.

(EMA-P038-2017) Nonlinear box-counting dimensions of grain cluster boundary and dielectric permittivity

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Correlation between rare-earth and other additives and substructure-microstructure properties for doped BaTiO_3 -ceramics and electronics properties, is presented. The grain contacts geometry based on granularity contact surface in terms of the generalized, nonlinear fractal morphology given. The main conclusion was that granularity capacities have changeable values then expected which is induced by contact surfaces sizes augmentation as a consequence of their generalized fractal, box size dependent nature. The effect of increasing capacity due to fractality of contact zone is referred to by these authors as the alpha-correction of the intergranular capacity or, what is the same, dielectric constant. Whereas the powder material is porous, there are two aspects of such a material fractality: the positive space made by grains collection and the negative space which is holes and pores collection. Ceramics materials during the sintering process change their inner morphology by shrinking pores and increasing solidity and compatibility. In this poster presents the box-counting scale dependent generalized method for determination new dimensions for nonempty compact subset in Euclidean space.

(EMA-P039-2017) Grains cluster boundary fractality and micro capacitors

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The broad ceramics capacitors application based on barium-titanate, demands a constant research of its structure. Intergranular structure and dielectric properties of ceramics depend on grains cluster boundary configuration. In the porous powder material, two aspects of cluster fractality have been observed: the negative space which is collection of holes (pores) and the positive space made by collection of grains. Several types of the Minkowski hull are known in the literature: average, local, essential week limited etc. For usual Minkowski hull, it is possible to have six intergranular connection types. For the proposed concept of the generalized Minkowski contents, with the corrected degree diameter (scale depend diameter), exists new ways to contact of the ceramic grains in the cluster, between maximums and minimums of the grain boundaries. This approach directly affects description of the surface area energy reduction and concept of working temperature of BaTiO_3 -ceramics, i.e. its dielectric and conductive properties. Since the REE (REM) additives may increase fractality, a systematic study of REE-fractal dimension relationship may open the gate to ceramic supercapacitors.

(EMA-P040-2017) Oxygen partial pressure effect on Wulff Shapes of Barium Titanate/Strontium Titanate Alloys

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The effect of oxygen partial pressure during sintering on the Wulff shape of alloys of barium titanate with strontium titanate is being studied. The perovskites BTO and STO form complete solid solutions across their entire compositional range. The oxygen partial pressure during sintering has an effect on the number of oxygen vacancies in the crystal. It is expected that changing the concentration of oxygen vacancies will affect grain growth and this effect can be observed in the Wulff shape. The Wulff shapes of 25 BTO: 75 STO and 75 BTO: 25 STO have been reconstructed from experimental pore shapes, making it possible to observe the transitions of the Wulff shape with changing composition. These have implications for surface segregation and grain growth.

(EMA-P041-2017) Growth and Electronic Structure Characterization of a $(\text{SrCoO}_x)_1:(\text{SrTiO}_3)_1$ Superlattice

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We report on the synthesis of a $(\text{SrCoO}_x)_1:(\text{SrTiO}_3)_1$ superlattice by oxide molecular beam epitaxy and the characterization of its electronic structure by soft x-ray spectroscopy. X-ray photoelectron and absorption spectroscopy reveal that Ti remains octahedrally coordinated with a 4+ oxidation state, while the Co oxidation state is intermediate of 3+ and 4+. Despite having the same half an oxygen vacancy per Co atom found in brownmillerite $\text{SrCoO}_{2.5}$, which consists of alternating tetrahedral and octahedral layers of Co, the confinement of oxygen vacancies to isolated single atomic layers of SrCoO_x stabilizes square pyramidal coordination of Co, as observed by the linear dichroism in the Co 2p-3d x-ray absorption. The corresponding stabilization of Co^{4+} along with Co^{3+} give rise to metallic behavior within the square pyramidal $\text{SrCoO}_{2.5}$ layers as indicated by a Fermi-edge step observed at strong Co 2p-3d resonance in the resonant photoemission spectroscopy of the valence band. This metallic behavior, along with a band gap of 1.7 eV, suggest the superlattice may be well-suited for photocatalysis. The obtained results demonstrate artificial superlattices as effective means to defect engineer complex oxides by harnessing the confinement of oxygen vacancies to control the oxygen coordination environment of the transition metal.

(EMA-P042-2017) Negative resistance in thin carbon films and graphite samples

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Recently, the negative resistivity observed in graphene was attributed to the viscous flow of electrons causing them to move contrary to the applied voltage. The observation of apparent negative resistance in composite materials leads to possible new areas of research, described by some as structural electronics. One such application is resistive random access memory devices. We are here studying the negative resistance properties of amorphous (a-C), diamond-like carbon (DLC) thin films, and graphitic samples such as PAN-derived fibers and (bulk) pyrolytic graphite discs that undergone oxygen-ion implantation at levels from 7.07×10^{12} to 2.24×10^{16} ions/cm². PPMS magnetoresistance measurements were conducted using the four-wire arrangement, for temperatures from 1.9 or 5 to 300 K and magnetic fields up to 9 T. In addition, Raman studies traced the amorphization trajectory (the position of the G peak and the I(G)/I(D) intensity ratio) in samples ranging from graphitic to a-C and DLC, as well as effects due to different levels of oxygen ion implantation. The resistivity becomes almost asymptotically large, either positive or negative, at temperatures that are sample- and/or implantation level- dependent. One such temperature is ~150 K. Our results show clearly that the oxygen-ion implantation leads to both negative resistivity and giant magnetoresistance observed in these carbon-based samples.

(EMA-P043-2017) Synthesis and Characterization of zircote magnetic ferrofluid for the application of the hyperthermia treatment

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We report the preparation of monophasic Zr-substituted magnetite ($\text{Zr}_x\text{Fe}_{3-x}\text{O}_4$; $0 < x < 1$) nanoparticles by wet chemical route. Such a report is lacking in the literature. Rietveld refinement of the X-ray diffraction (XRD) data suggests continuous decrease in the lattice parameter with increased Zr-substitutions. From TEM analysis, the size of the as synthesized particles was found to be in the range of 5–20 nm. The differential scanning calorimetry (DSC) curves for the samples with different amount of substitutions displayed

considerable differences in their behaviors. The room temperature specific magnetization at 2 T has been found to decrease from 50 ($x \approx 0.2$) to 41 A m²/kg ($x \approx 1.0$) with increased Zr-substitution. From XRD and magnetic behavior analysis we could suggest that due to occupation of Zr^{4+} ions at tetrahedral and octahedral voids of Fe_3O_4 , the amount of Fe^{2+} was more at octahedral site for $x < 0.4$ and at tetrahedral site for $x > 0.4$ respectively. The ferrofluids prepared from these magnetic nanoparticles possessed good heating ability and Specific Absorption Rate (SAR) values suitable for hyperthermia treatment.

(EMA-P044-2017) Local structure studies of disordered and nanocrystal ferroelectrics

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As materials become increasingly complex and the miniaturization of functional materials continues, the ability to characterize intricate structural details is key to developing robust structure-property relationships. This poster highlights several cases where local structure probes (total scattering and pair distribution functions, PDFs) have revealed nanoscale structural features that are otherwise inaccessible. One such example is the application of neutron total scattering to ferroelectric oxide nanocrystals (e.g., BaTiO_3) to investigate the effects of particle shape, size, and surface termination on the “internal” crystal structure. Neutron PDFs are sensitive to indications of either stabilization or destabilization of polarization for small nanocrystals including Ti-O bond length distributions and the degree of correlation of ferroelectric distortions. This methods is also well-suited for elucidating structural features of disordered ferroelectrics including Bi- and Pb-based solid solutions (e.g., BiScO_3 - PbTiO_3 , BaTiO_3 - $\text{Bi}(\text{M}^{3+})\text{O}_3$, $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ -based, etc.) This poster showcases the suitability of the Nanoscale-Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source at Oak Ridge National Laboratory for such experiments. We will also demonstrate some new methods and advanced toolsets we have developed to address the emerging challenges of modeling complex nanomaterial systems.

(EMA-P045-2017) Photovoltaic Effect in VO_2 nano-island/ BiFeO_3 heterostructure

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Semiconducting ferroelectrics, which possess a spontaneous and switchable electric polarization with suitable band-gap, have recently attracted interest for photovoltaic applications. A large electric polarization can promote the desirable separation of photo-excited carriers. However, ferroelectric photovoltaic performances are often limited by poor conduction and unsuitable interface for realizing charge carrier separation. We fabricated VO_2 nano-island on BiFeO_3 thin film by pulsed laser deposition. BiFeO_3 is ferroelectric material that has a band-gap (~2.7 eV) enable to harvest visible-light. VO_2 undergoes a first-order metal-insulator transition (MIT) at a critical temperature (~340 K). The transition involves drastic change in both electric resistivity and crystal structure. For VO_2 nano-island/ BiFeO_3 structure, photovoltaic performance is strongly sensitive to the phase transition of VO_2 . At room temperature, semiconducting VO_2 nano-island works as hole injection layer to increase photo charge carrier. Above the critical temperature, plasmonic effect of metallic VO_2 nano-island can improve the photovoltaic performance in the structure. MIT nano structure can provide a key to enhancing photovoltaic effect in oxide heterostructure.

(EMA-P046-2017) Nanostructured ZnO/graphene for hybrid supercapacitor devices

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The development of complementary energy storage devices has been study in the last years. Efforts have been made to satisfy the requirements of electrochemical energy storage, such as supercapacitors, using materials with high cost-benefit relation. Transitions metal oxides, like ZnO, are promising materials for supercapacitors due to their excellent pseudocapacitive properties, fast and reversible redox reactions. Graphene, on the other hand exhibits high electrical conductivity and suitable double layer properties for supercapacitors. In this work, ZnO/graphene nanocomposites were produced by sol-gel process. Graphene was incorporated in situ in different concentrations, from 3 wt.% to 10 wt.%(relative to the precursor, ZnCl₂). Supercapacitors were assembled using the nanocomposites as active electrodes and PVA/H₃PO₄ as gel electrolyte. The device mounted with pure ZnO presented specific capacitance of 19 F/g. Incorporation of graphene provided a double layer capacitance in addition to the pseudocapacitance of the ZnO. The ZnO/3%graphene device presented a capacitance of 423F/g, while the ZnO/5% graphene presented 378F/g. Addition of 10%graphene, however decreased the specific capacitance to 161F/g. The device assembled with ZnO/ 3%graphene presented values of energy density and power density that classify them in the supercapacitor category, delivering a maximum energy density of 2.5Whkg⁻¹ and a maximum power density of 96kWkg⁻¹.

(EMA-P047-2017) WO₃ anstructures synthesized via microwave-assisted hydrothermal methods

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Tungsten oxide (WO₃) is one of the interesting materials for wide applications in electrochromic devices, photo-catalysts, and gas sensors. For those applications, several attempts have been made in the synthesis of WO₃, such as structural modification, doping of various elements and morphology changes. Nanostructures of WO₃ have superior properties compared with its bulk structures. In this presentation, hexagonal WO₃ nano-rod structures have been studied by using scanning electron microscopy (SEM), X-ray diffraction, BET techniques, and UV-vis spectroscopy for morphology, structure, surface area, and band-gap measurements, respectively. The microwave-assisted hydrothermal methods were used to fabricate nanofiber structures by adding oxalic acid in the process of the preparation of solution. The tungsten precursor of Na₂WO₄·2H₂O were dissolved in double distilled water. The control of pH was adjusted by adding diluted HCl solution. After adding a directiona agent, the resulting mixture was transferred to a hydrothermal reaction autoclave. The duration time and heating temperature during the hydrothermal synthesis are 30~60 min and 120°C at various power conditions, respectively. The obtained WO₃ powder showed single phase hexagonal structure, 20-40 nm diameter and 1-2 mm long nano-rod bundles.

(EMA-P048-2017) The large room temperature perpendicular exchange bias in the self-assembled NiO-NiFe₂O₄ nanocomposites

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The exchange bias (EB) effect with perpendicular anisotropy has attracted continuous attention due to potential applications in high-density magnetic storage devices, such as the giant magnetoresistance (GMR) read head. In the vertical aligned heteroepitaxial nanocomposites (VHN), the large amount of interfaces and the out-of-plane shape anisotropy can result in a large perpendicular EB theoretically. However, due to the limited choices of antiferromagnetic and ferromagnetic materials in the VHN and the special requirements of the EB on the magnetic ordering temperatures and anisotropies of both materials, the reported EB in the VHN are

either at very low temperature or of small magnitude. These drawbacks largely limit the application of EB in devices. In this work, a large perpendicular EB of 0.85 kOe at room temperature is realized in the self-assembled NiO-NiFe₂O₄ nanocomposites grown on SrTiO₃(001) substrate with pulsed laser deposition. A very high Curie temperature of NiFe₂O₄ (T_C~790 K) and Néel temperature of the NiO (T_N~525 K) with T_C>T_N can induce EB with blocking temperature far above room temperature. More interestingly, the EB shows a significant dependence of different substrates. When deposited on the MgO(001) substrate, the nanocomposites shows no EB due to the spin compensation of the well-formed interfaces between these two phases with very good crystalline.

(EMA-P049-2017) Electrophoretic deposition of magnesium diboride

W. Straka^{*1}; J. Schwartz¹; 1. North Carolina State University, USA

Magnesium diboride shows promise for replacing low temperature superconductors for some magnetic applications due to its high critical temperature and relatively high critical current density in comparison to Nb₃Sn and NbTi. The most common way of synthesizing MgB₂ wires is through the powder-in-tube (PIT) process. This often includes multiple steps to achieve fully dense wires including enormous pressures. One potential synthesis route for creating MgB₂ wires is to use electrophoretic deposition (EPD). This technique uses an electric field to physically deposit MgB₂ powder from suspension on a conductive substrate. Through this technique, complex geometries can be coated and allows for quick addition of dopants to improve low field properties. Electrical and magnetic results from deposition of MgB₂ films on various conductive wires will be shown. Microscopy images will be used to verify the density of the wires.

(EMA-P050-2017) Calorimetric Measurements of AC Loss of YBCO Conductors and Cables at High dB/dt in a Stator Environment

T. J. Haugan^{*1}; J. P. Murphy²; M. Sumption³; T. Bullard⁴; N. Gheorghiu⁴; 1. U.S. Air Force Research Laboratory, USA; 2. University of Dayton Research Institute, USA; 3. The Ohio State University, USA; 4. UES Inc., USA

A new facility for the measurement of AC loss in superconductors at high dB/dt has been developed, and recently tested and calibrated for operation. The test device has a spinning rotor consisting of permanent magnets arranged in a Halbach array; which exposes samples in a stator position with a peak radial field of 0.57 T, and with high rotation speeds up to 3600 rpm achieves a radial dB/dt is 543 T/s and tangential dB/dt is 249 T/s. Loss is measured by calorimetry using nitrogen boiloff from a double wall calorimeter feeding a gas flow meter, and the system was calibrated using power from a known resistor. Herein the use of this system for measuring AC losses of a variety of YBCO coated conductors and cables will be performed, and results will be compared to measurements with a a solenoid magnet system and theory. Coated conductors are provided by several manufacturers with different architectures including filamented, varying width, and different quench protection metal layers with varying thickness. Also AC losses will be reported on several types of cable structures, including stacked tapes and conductor-on-round-core (CORC) structures. Acknowledgements: The Air Force Office of Scientific Research (AFOSR), The Air Force Research Laboratory - Aerospace Systems Directorate (AFRL/RQ)

(EMA-P051-2017) Investigation of Hetero-structure Formation and Interface Property of Bi2212 and Topological Insulator

C. Rong^{*1}; P. J. Taylor¹; P. A. Folkes¹; D. M. Potrepka¹; P. N. Barnes¹; 1. U.S. Army Research Laboratory, USA

We report some of the recent results of experimental investigation on hetero-structures formed by Bi2212 with a topological insulator Pb_{0.5}Sn_{0.5}Te. Bi2212 was heat processed to form a textured structure with crystal lattice alignment along the c axis. Crystalline Pb_{0.5}Sn_{0.5}Te was subsequently grown by MBE on top of the textured

superconductor. Structural, electric, and magnetic characterization techniques were employed to probe the electronic state at the interface, including the possible proximity effect reported in the literature. Knowledge gained from this study has potential for significant device applications in advanced electronics and next-generation computing.

(EMA-P052-2017) An Investigation of the Superconducting Properties of the beta-Mn ($T_{1-x}R_x$)₃Al₂C solid solutions

M. A. Susner^{*3}; T. Bullard³; M. Sumpston¹; T. J. Haugan²; 1. The Ohio State University, USA; 2. U.S. Air Force Research Laboratory, USA; 3. UES, Inc., USA

Recently interest in the superconducting community has been piqued by superconducting materials that have a non-centrosymmetric crystal structure in which spin singlet or spin triplet states can develop. In this study we investigate the cubic beta-Mn system ($T_{1-x}R_x$)₃Al₂C (T,R = Mo, Nb, Ta, V, Ti, Cr, Sc) by systematic replacement of the T element of the compound. Of the end member compounds only T = Nb and Mo are known to superconduct at 1.3K and 9.2K respectively. By doping the Mo system we hope to further elucidate these unique pairing states as well as enhance T_c . The above-named compositions were investigated via magnetic, resistive, and calorimetric analyses. The superconducting phase diagrams of these compounds were then plotted. Comparisons are made between the effects of doping different transition metal elements as well as possible substitutions on the Al and/or C sites.

Thursday, January 19, 2017

Plenary II

Room: Indian

Session Chair: Rick Uvic, Boise State University

8:40 AM

(EMA-PLEN-002-2017) From Ultra-High Q dielectrics to the room temperature MASER

N. McN. Alford^{*1}; 1. Imperial College, United Kingdom

In this talk we will look at the problem of dielectric loss (the $\tan \delta$) in oxides and specifically methods to beat the dielectric limit. We do this using a Bragg reflector in which the Bragg layers, which are made of sapphire, are of equal thickness. In this case the Q factor (or the inverse of the $\tan \delta$) saturates to a plateau after around 3 layers. Surprisingly we find that if the layers are aperiodic in thickness there is no saturation and the Q factor rises quadratically to reach remarkably high values of $Q=0.6 \times 10^6$ at 30GHz. This result suggested that it might be possible to reach the threshold for masing and indeed we demonstrated recently that in P-terphenyl doped with pentacene when located inside a very high Q sapphire resonator maser action can be observed. This is the first time a solid state maser has been demonstrated at room temperature and in the earth's magnetic field. Recent work has shown that miniaturisation is feasible and considerable reduction in pumping power is possible by using a strontium titanate resonator which by virtue of a higher relative permittivity leads to a factor of over 5 in size reduction. Importantly, the Purcell factor which is the ratio of the Q factor to the mode volume, remains high and this is a key factor in the ability to exceed the threshold for masing.

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Advanced Electronic Materials: Piezoelectric

Room: Indian

Session Chairs: Zuo-Guang Ye, Simon Fraser University; Jun Luo, TRS Technologies, Inc.

10:00 AM

(EMA-S1-018-2017) Exploring the Structures and Properties of Novel Piezo-/ferroelectric Single Crystals (Invited)

Z. Ye^{*1}; 1. Simon Fraser University, Canada

Recent efforts have been put in the development of high-performance piezo-/ferroelectric crystals that can overcome the drawbacks of the PMN-PT-based binary crystals suffering from low Curie temperature (T_C) and low depoling temperature (T_{RT}). In this talk we present the phase symmetry, domain structure and physical properties of PIN-PMN-PT-based (Generation II) piezocrystals and some new ternary systems. To explore the piezocrystals beyond Generation II, we have grown and characterized the ferroelectric crystals of new PMN-PSn-PT ternary system which exhibit high piezoelectricity (with $d_{33} = 1400$ pC/N) without undergoing any poling process and showing a piezoelectric memory effect. This uncommon piezoelectric effect is explained by a self-polarization mechanism based on the defect-dipoles due to the presence of mixed valence states of $Sn^{2+/4+}$. The defect-dipoles generate internal bias fields which, in turn, provide the stabilizing and restoring forces leading to preferred orientation and retention of spontaneous polarization. This mechanism offers a new perspective for designing novel piezoelectric materials with high performance and a wide temperature range of operation.

10:30 AM

(EMA-S1-019-2017) Relaxor-PT ferroelectric crystals and their applications in diagnostic medical ultrasound imaging (Invited)

J. Luo^{*1}; S. Taylor¹; S. Zhang²; 1. TRS Technologies, Inc., USA; 2. University of Wollongong, Australia

This talk reviews the recent development of binary and ternary relaxor-PT piezoelectric single crystals with emphasis on the crystal growth, characterization and their diagnostic medical transducer applications. For ferroelectric piezoelectric materials, $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) ceramics with composition near the morphotropic phase boundary (MPB) have been the mainstay for the transducer fields since 1950's. Development of the relaxor-based ferroelectric crystals of $Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ (PMN-PT) and $Pb(Zn_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ (PZN-PT) represents a revolutionary advance for piezoelectric applications. These binary relaxor-PT crystals provide several key advantages over PZT ceramics, including high elastic compliances (4-5 times of PZT), large piezoelectric coefficients (3-5 times of PZT), and extremely high electromechanical coupling coefficients ($k_{33} > 90\%$). By B-site substitution, ternary crystals, such as $Pb(In_{1/2}Nb_{1/2})O_3$ - $Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ (PIN-PMN-PT), and Mn doped ternary crystals, such as Mn:PIN-PMN-PT, have largely expanded the operational temperature and electric field. A broad range of applications for diagnostic medical ultrasound transducers either have been commercialized or are in great interest of research.

11:00 AM

(EMA-S1-020-2017) Simultaneous Field and Stress Control of Ferroelectric Phases in PIN-PMN-PT (Invited)

P. Finkel^{*1}; M. Staruch¹; M. Ahart²; A. Amin²; S. Lofland³; 1. U.S. Naval Research Laboratory, USA; 2. Naval Undersea Warfare Center, USA; 3. Rowan University, USA; 4. Carnegie Institute of Washington, USA

Relaxor ferroelectric single crystals with composition near a morphotropic phase boundary (MPB) are attractive for applications in actuators, transducers, and low-power sensors due to their extremely large piezoelectric response. This MPB can be moved through the application of stress or electric field. In this work we demonstrate an induced rhombohedral (R) to orthorhombic (O) phase transition in [011] cut $\text{Pb}(\text{In}_{1/2}\text{Nb}_{1/2})\text{O}_3$ - $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - PbTiO_3 (PIN-PMN-PT) single crystal relaxor ferroelectric, that can be simultaneously tuned through combination of stress and applied electric field. Direct observations of this phase transition with X-ray and Raman scattering reveal the local symmetry while sweeping through the transition with a low applied electric field when the crystal is near a critical value of stress. A coexistence of R and O phases was observed and these microscopic measurements mirror the bulk strain in the sample. Remarkably, cycling through this transition can generate reversible strain >0.35% for tens of millions of cycles with little fatigue. Details of these results and their implications will be presented.

11:30 AM

(EMA-S1-021-2017) Investigation of the aluminum nitride - scandium nitride alloy system for piezoelectric applications

K. R. Talley^{*1}; G. L. Brennecke¹; A. Zakutayev²; A. Holder²; S. Millet³; 1. Colorado School of Mines, USA; 2. National Renewable Energy Laboratory, USA; 3. University of Colorado, Boulder, USA

This work investigates piezoelectric aluminum/scandium nitride alloys in the film bulk acoustic resonator (FBAR) application space through the combination of energy calculations and experimental deposition and characterization. The (Al/Sc)N material system has been the target of various investigations due to an enhanced piezoelectric response compared to pure aluminum nitride, the dominant material used in these devices. Mixing energy calculations show a low solubility limit of scandium in aluminum nitride and a strong driving force for phase separation. However, kinetically trapped phase stability has been observed to ~30% ScN alloying. Al(1-x)Sc(x)N films were produced through combinatorial reactive co-sputtering from metallic targets and deposited atop silicon p(100) substrates, where $0 \leq x < 0.5$. The alloyed films were screened for the structure, composition, and thickness, as well as the modulus of elasticity, piezoelectric coefficient, and electrical permittivity as the relevant properties that contribute to the figure of merit for FBAR devices. The structure and phase evolution of the resulting films is analyzed and compared to the changes observed in the properties of interest.

11:45 AM

(EMA-S1-022-2017) Giant piezoelectric voltage coefficient in grain oriented modified-PbTiO₃ material

Y. Yan^{*2}; J. Zhou¹; D. Maurya²; Y. Wang¹; S. Priya²; 1. Michigan Tech, USA; 2. Virginia Tech, USA

A rapid surge in the research on piezoelectric sensors is occurring with the arrival of the Internet of Things (IoTs). Single-phase oxide piezoelectric materials with giant piezoelectric voltage coefficient (g, induced voltage under applied stress) and high Curie temperature (T_c) are crucial towards providing desired performance for sensing, especially, under harsh environmental conditions. Here, we provide rational design criterion for such piezoelectric sensing material by incorporating (a) anisotropy/composition/phase structure, (b) microstructure and (c) domain engineering. Using this criterion we report a grain-oriented (with 95% <001> texture) modified-PbTiO₃ material that has a high T_c (~364°C) and an extremely large g₃₃ (115 × 10⁻³ Vm/N) in comparison to other known single

phase oxide materials. Diffraction and scanning probe microscopy studies reveal that self-polarization due to grain orientation along the spontaneous polarization direction plays an important role in achieving large piezoelectric response in a domain-motion-confined material. Domain-level mechanisms were verified quantitatively by simulations using phase field model. The simulations confirm that the large piezoelectric voltage coefficient g₃₃ originates from maximized piezoelectric strain coefficient d₃₃ and minimized dielectric permittivity ε₃₃ in [001]-textured PbTiO₃ ceramics where domain wall motions are absent.

12:00 PM

(EMA-S1-023-2017) Mechanical characterization of LiTaO₃ and LiNbO₃ single crystals for application as surface acoustic wave filters

M. Gruber^{*1}; D. Kiener²; P. Supancic¹; R. Danzer¹; R. Bermejo¹; 1. Montanuniversitaet Leoben, Austria; 2. Montanuniversitaet Leoben, Austria

Lithium tantalate (LiTaO₃) and lithium niobate (LiNbO₃) possess various attractive properties such as piezo-electricity, making them interesting for surface acoustic wave (SAW) filter substrates for high frequency data transfer. Although appropriate functional characterization of these materials can be found in literature, a lack of knowledge exists regarding the mechanical properties of these single crystal components. In this work, the mechanical behaviour of LiTaO₃ and LiNbO₃ single crystals was assessed in terms of strength and fracture resistance with respect to the cutting direction and the surface quality. The biaxial strength was evaluated on plate-like specimens cut from a wafer, using the ball-on-three-balls test. The fracture response was analysed using spherical nanoindentation and in-situ tests of FIB-notched micro cantilevers to quantify fracture toughness of the most critical cleavage planes. Experimental findings showed a significant difference in strength between LiTaO₃ and LiNbO₃. A deviation from Weibull statistics was observed in LiNbO₃. Fractography of the tested samples showed differences in the fracture patterns, which are explained by the different fracture toughness and cutting orientation of the two investigated materials.

12:15 PM

(EMA-S1-024-2017) Development of Texture in PMN-PZT Piezoelectric Ceramics and Their Ultrasonic Motor Applications

S. Alkoy^{*1}; S. Dursun¹; E. Mensur-Alkoy²; 1. Gebze Technical University, Turkey; 2. Maltepe University, Turkey

High power piezoelectric materials combine “hard” and “soft” electrical characteristic for device applications such as ultrasonic motors, transformers and medical ultrasound. Therefore, piezoelectric materials with a high mechanical quality factor (Q_m) is desirable to meet the high power requirement, and high piezoelectric constant and electromechanical coupling are required for improved strain performance. In this study, combination of two approaches has been used to obtain the high power characteristics, namely; texturing to increase “soft” characteristics and Mn-doping to obtain “hard” characteristics. Textured 0.4Pb(Mg_{1/3}Nb_{2/3})O₃-0.25PbZrO₃-0.35PbTiO₃ (PMN-PZT) piezoceramics with properties that are comparable to single crystals in certain crystallographic directions were synthesized by Templated Grain Growth (TGG) method using BaTiO₃(BT) template particles. Textured PMN-PZT ceramics with Lotgering factors of up to 0.85 and with % 1.5 mol MnO₂ doping exhibited hard and soft combinatory properties with piezoelectric coefficients of d₃₃ = 600 pC/N, k_p=0.78, tand=0.3 %, K^T=1320 and Q_m=550. The high power performance of textured PMN-PZT was also successfully demonstrated in an ultrasonic motor with a cubic stator geometry. The authors would like to thank the financial support of the Scientific and Technical Research Council of Turkey (TUBITAK) through the Project #114M518.

S2: Advanced Processing for Electronic and Electrochemical Systems: Crystals, Films and Devices

Functional Materials: Synthesis Science, Properties, Integration

Room: Coral B

Session Chair: Jon Ihlefeld, Sandia National Laboratories

10:00 AM

(EMA-S2-019-2017) Comparison and Evaluation of Mn Doped PZT Thin Films for Resonant PiezoMEMS Devices

R. G. Polcawich^{*1}; R. Q. Rudy¹; K. Grove¹; 1. US Army Research Laboratory, USA

In the continued advancement of piezoelectric MEMS (PiezoMEMS) technology, improvements in thin film deposition and patterning and improved processing control are crucial to enabling high yield process flows. This presentation will compare Mn doped lead zirconate titanate (PZT) thin films for possible use in resonant based PiezoMEMS devices. Specifically, chemical solution deposition was used to process (001) textured PZT (52/48) thin films followed by a surface micromachining fabrication process to create clamped circular capacitors, unclamped cantilevers, and unclamped length extensional and flexure mode resonators. Preliminary results agree with previously published reports indicating a doping level of approximately 4% Mn yields a minimum in the dielectric constant and dielectric loss tangent while maintaining a reasonable remnant polarization. Using these preliminary numbers, piezoelectric coefficient values and resonator performance are currently being evaluated to determine if the reductions in dielectric properties result in substantial improvements in PiezoMEMS resonant devices.

10:15 AM

(EMA-S2-020-2017) Measurement and Modelling of effective piezoelectric coefficients of thin films

M. Sivaramakrishnan^{*1}; P. Mardilovich²; T. Schmitz-Kempen³; S. Tiedke³; 1. Xaar, United Kingdom; 2. Xaar, United Kingdom; 3. Aixacst, Germany

Integration of piezoelectric thin films in a standard MEMS process is an attractive new technology for many applications. Reliable, precise and repeatable characterization of piezoelectric performance of thin films is essential for the comparison of materials prepared under different processing conditions. It is well known that the clamping of the piezoelectric film to a semi-rigid substrate makes the determination of piezoelectric coefficients of thin films more challenging. Modelling plays a key role in the understanding of the role of substrate effects and to relate the measured quantities to the intrinsic properties of the material. The effective longitudinal piezoelectric coefficient ($d_{33,f}$) is measured by double beam laser interferometry (DBLI) and the transverse effective piezoelectric coefficient ($e_{31,f}$) can be measured on singularized bending beams or cantilevers or on full wafers. It is also important to distinguish between large-signal and small signal piezoelectric coefficients. Additionally, in the case of ferroelectric films, hysteresis, poling, imprint and sample history also lead to significant differences in the measured quantities. In this talk we will present a comprehensive review of the status of the measurement and modelling of piezoelectric performance of thin films.

10:30 AM

(EMA-S2-021-2017) Improved Performance and Reliability in (001) Textured PZT Films for PiezoMEMS through Compositional and Doping Profiles

T. M. Borman^{*1}; W. Zhu¹; S. Ko²; P. Mardilovich²; S. Trolier-McKinstry¹; 1. Pennsylvania State University, USA; 2. Xaar, United Kingdom

Strongly {100}/(001) textured $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ (PZT52/48) films were deposited utilizing Mitsubishi Materials Corporation E1 sol-gel solutions on substrates platinized at 500°C by sputter deposition. Gradient "free" films were achieved via use of three solutions of average Zr/Ti composition 52/48. Compositional profiles including additional Ti rich layers were utilized in conjunction with tailored manganese (1%) and niobium (2%) doping. Films were oriented using PZT seed layers which were pyrolyzed at 300°C and crystallized at 700°C under low ramp rates (10°C/s) and O_2 gas flow (2 slpm). Bottom electrodes made from Pt deposited at temperatures of 500°C or more facilitate growth of PZT with less pyrochlore and a lower nucleation density than films grown on platinum deposited at room temperature. ~1.5 μm thick films grown with lead excess levels of 14 to 16 atomic percent in all layers were found to be dense with limited pyrochlore formation. Despite the high lead content of the solutions, leakage currents were on the order of 10^{-8} A/cm² at room temperature and 10^{-5} A/cm² at 200°C under an applied field of 10E_c. Rayleigh analysis demonstrates an increase in the irreversible contributions to domain wall motion from niobium doping. Finally, the piezoelectric properties of poled films with different composition profiles will be discussed.

10:45 AM

(EMA-S2-022-2017) Normal and Lateral Enhancement of Piezoactuation for Geometrically Strain Relieved Functional Microstructures

L. Ye¹; R. Keech²; R. Cordier¹; S. Trolier-McKinstry²; B. D. Huey^{*1}; 1. University of Connecticut, USA; 2. Pennsylvania State University, USA

Microfabrication of functional materials into discretely addressable elements is integral to a wide range of devices including actuators, switches, transistors, filters, and logic elements. With device scaling, however, the edge to bulk ratio for individual microfabricated features increases. This has potential implications for the performance and reliability of each element. For strained piezoelectrics, for example, geometrically relieved edges may approach bulk-like properties. This is confirmed with strained PMN-PT thin films using PFM, both in the normal as well as lateral directions. Specifically, the piezoresponse is enhanced as a function of distance from the free edge up to ~500 nm, and depending on the dimensions of the micro-fabricated structure for submicron features.

11:00 AM

(EMA-S2-023-2017) "Ferroelectricity" in epitaxial $\text{Pb}_{1+\delta}\text{ZrO}_3$ thin films

R. Gao^{*1}; S. R. Lillo²; R. Xu¹; L. Dedon¹; Y. Dong³; H. Zhou³; A. Dasgupta¹; Z. Chen¹; C. R. Serrao⁴; J. Neaton²; L. W. Martin¹; 1. University of California, Berkeley, USA; 2. University of California, Berkeley, USA; 3. Advanced Photon Source, Argonne National Laboratory, USA; 4. University of California, Berkeley, USA

The antiferroelectric PbZrO_3 is being considered for a wide range of applications where the competition between polar and non-polar ground states is important. Here, we focus on the epitaxial growth of PbZrO_3 thin films and understanding the chemistry-structure coupling in stoichiometric, 10% Pb-excess, and 20% Pb-excess versions of PbZrO_3 . Using RHEED-assisted pulsed-laser deposition, we are able to achieve continuous 2D growth of high-quality, single phase films with nominal chemistries of $\text{Pb}_{1+\delta}\text{ZrO}_x$ ($\delta=0, 0.1, 0.2$) as further confirmed by RBS studies. DFT calculation and XANES studies suggest that the large cation nonstoichiometry is accommodated by the creation of Pb-antisite defects. Electrical characterization reveals that while the PbZrO_x and $\text{Pb}_{1.1}\text{ZrO}_x$ remain

antiferroelectric in nature, the $\text{Pb}_{1.2}\text{ZrO}_x$ exhibits single ferroelectric-like hysteresis loop with a remnant polarization of $10 \mu\text{C}/\text{cm}^2$. Further scattering studies show 450° -diffraction peak in PbZrO_x and $\text{Pb}_{1.1}\text{ZrO}_x$, while no such peak is observed for $\text{Pb}_{1.2}\text{ZrO}_x$ confirming the absence of antiferroelectric displacements of the Pb atoms. The calculations suggest a polar phase belonging to the $R3c$ space group, in particular in the presence of Pb-antisite defects. In the end, the possibility of deterministically-controlling the ground state of PbZrO_3 through growth and defect engineering sheds new insights into the nature of electrical response in materials.

11:15 AM

(EMA-S2-024-2017) Thickness Dependence of Polarization and Electronic Conduction in $(\text{Hf,Zr})\text{O}_2$

S. W. Smith^{*1}; A. Kitahara¹; M. Rodriguez¹; D. Henry¹; M. Brumbach¹; J. Ihlefeld¹; 1. Sandia National Laboratories, USA

$(\text{Hf,Zr})\text{O}_2$ is an exciting, recently discovered ferroelectric that can be deposited as a thin film by atomic layer deposition. $(\text{Hf,Zr})\text{O}_2$ is unusual because its ferroelectric response is due to a metastable phase most commonly seen as a thin film and its polarization response has been shown to increase with decreased thickness, at size scales that are unusual for conventional ferroelectric materials. Still, like more traditional ferroelectrics, properties are expected to degrade at some point, as the thickness approaches that of a single unit cell. The surface limited growth of atomic layer deposition is a natural fit for producing the very thin films needed to investigate this thickness regime. In this work we will explore the impact thickness has on polarization and on conduction through thin ($<20 \text{ nm}$) $(\text{Hf,Zr})\text{O}_2$ films in the context of preparing ferroelectric tunnel junction devices. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:30 AM

(EMA-S2-025-2017) Alternative spray-based processing methods for dielectric and piezoelectric film deposition

M. Deluca^{*1}; R. Wimmer-Teubenbacher¹; M. Bruckner²; J. Kita²; R. Moos²; K. Reichmann³; G. A. Maier¹; 1. Materials Center Leoben Forschung GmbH, Austria; 2. University of Bayreuth, Germany; 3. Technische Universitaet Graz, Austria

Ferroelectric thin and thick films are widely used for energy harvesting and energy storage applications. Processing methods like sputtering, physical/chemical vapor deposition or chemical solution deposition (CSD) are generally used, whereby the latter has the advantage of lower cost and high flexibility with respect to the achievable range of microstructure, composition and properties. CSD methods, however, require repetition of deposition-pyrolysis-crystallization cycles to achieve desired thicknesses up to and above $1 \mu\text{m}$. In this work, we explore the possibilities offered by two alternative deposition methods: Aerosol deposition, in which a calcined powder is sprayed at high velocity onto a substrate and consolidates upon impact, and spray pyrolysis, a CSD method in which a precursor solution is sprayed on a hot substrate and pyrolyzes on contact. We used these methods to deposit BaTiO_3 films on both alumina substrates with Ag-based electrode and full sheet Cu-covered FR4 substrates. Film thicknesses up to $3 \mu\text{m}$ have been achieved. The structure and morphology of the prepared films were characterized with SEM, XRD and Raman spectroscopy. Furthermore, we characterized the dielectric and ferroelectric properties of the films, in order to clarify the potential of these deposition methods in obtaining properties comparable to those achievable with traditional processing routes.

11:45 AM

(EMA-S2-026-2017) Flexoelectric and flexocaloric Effects, Misfit Dislocations, and Strain Gradients: Electrothermal Properties of Ultrathin Ferroelectric Films

H. Khassaf^{*1}; T. Patel¹; P. S. Alpay¹; 1. University of Connecticut, USA

A non-linear thermodynamic analysis has been carried out to investigate the flexocaloric behavior of epitaxial ferroelectric thin films. We take into account the role of interface dislocations that generate strain gradients through the film thickness and thermal stresses. While misfit dislocations relax in-plane epitaxial strains, they also generate strain gradients localized to the film-substrate interface which in turn produce systematic polarization variations. We show here that the polarization gradients result in significant flexocaloric temperature variations in ultra-thin epitaxial ferroelectric films. More generally, our findings indicate that electrocaloric and pyroelectric properties of ferroelectrics can be supplemented with contributions from built-in stress fields and the flexoelectric effect.

12:00 PM

(EMA-S2-027-2017) Untangling Electrostatic and Strain Effects on the Polarization of Ferroelectric Superlattices

E. Khestanova¹; N. Dix¹; I. Fina¹; M. Scigaj¹; J. Rebled²; C. Magén³; S. Estradé²; F. Peiró²; G. Herranz²; J. Fontcuberta¹; F. Sanchez^{*1}; 1. Institut of Materials Science of Barcelona (ICMAB-CSIC), Spain; 2. Universitat de Barcelona, Spain; 3. Universidad de Zaragoza, Spain

The polarization of ferroelectric superlattices is determined by both electrical boundary conditions at the ferroelectric/paraelectric interfaces and lattice strain. The combined influence of both factors offers new opportunities to tune ferroelectricity. However, the experimental investigation of their individual impact has been elusive because of their complex interplay. Here, we present a simple growth strategy that has permitted to disentangle both contributions by an independent control of strain in symmetric $\text{BaTiO}_3/\text{SrTiO}_3$ superlattices. The superlattices were grown by pulsed laser deposition with real time control by reflection high energy electron diffraction. The out-of-plane parameter in fully coherent superlattices of a fixed period is controlled by the deposition rate. It is found that fully strained short period superlattices display a large polarization whereas a pronounced reduction is observed for longer multilayer periods. In comparison to the impact of the superlattice period, the effects of strain are relatively minor. These observations indicate that electrostatic boundary conditions fully dominate the ferroelectric response of the superlattices. It is also concluded that, a uniform ferroelectric entity, artificial-like ferroelectric material, is limited exclusively to ultra-short period superlattices.

S4: Computational Design of Electronic Materials

Materials by Design I

Room: Coral A

Session Chair: Mina Yoon, Oak Ridge National Laboratory

9:45 AM

(EMA-S4-001-2017) Rational Computation-Guided Design of Polymer Dielectrics (Invited)

R. Ramprasad^{*1}; 1. University of Connecticut, USA

To date, trial and error strategies guided by intuition have dominated the identification of materials suitable for a specific application. We are entering a data-rich, modeling-driven era where such Edisonian approaches are gradually being replaced by rational strategies which couple predictions from advanced computational screening with targeted experimental synthesis and validation. Consistent with this emerging paradigm, we propose a strategy of hierarchical modeling with successive down-selection stages

to accelerate the identification of polymer dielectrics that have the potential to surpass “standard” materials for a given application. Specifically, quantum mechanics based combinatorial searches of chemical and configurational spaces, supplemented with data-driven (machine learning) methods are used. These efforts have led to the identification of several new organic polymer dielectrics within known generic polymer subclasses (e.g., polyurea, polythiourea, polyimide), and the recognition of the untapped potential inherent in entirely new and unanticipated chemical subspaces offered by organometallic polymers.

10:15 AM

(EMA-S4-002-2017) Materials Modeling Applied to Enablement of Emerging and Scaling Memory Technologies (Invited)

S. C. Pandey^{*1}; 1. Micron Technology Inc., USA

As a technology evolves, computational simulations play a key role at several stages, from the basic materials research to estimates of device performance and reliability, to the development of fabrication processes enabling large-scale device integration to achieve chip-level functionality. Applications are presented of first-principles atomistic modeling that cover predictive screening, design, and optimization of ceramics for emerging memory devices (STT-RAM, MeRAM, ReRAM, PCM) as well as currently scaling (DRAM, NAND) technologies. Findings from multi-scale models consistent with experiments are discussed, which include charged defects/impurities in transition-metal and multi-valent oxides, and chalcogenide glasses incorporating interfacial physics critical to electrical performance. Few oxides are presented in terms of new size- and composition-dependent phases and transitions, which can be exploited as multifunctional tunneling barriers and capacitors. Electrical behavior is modeled to comprehend electron/spin/heat transport in imperfect materials, accounting for its composite nature, microstructure, and dimensionality. We also present screening study of thin-film deposition precursors to identify complexes conforming to process-induced constraints. Theoretical and computational challenges to achieving higher fidelity and throughput for technologically relevant systems are also outlined.

10:45 AM

(EMA-S4-003-2017) First-principles materials design of novel functional oxides (Invited)

V. R. Cooper^{*1}; 1. Oak Ridge National Laboratory, USA

Theory and computation are critical to the materials discovery process. Electronic structure methods excel at the characterization of macroscopic properties, while predicting synthesizability and operability is less straightforward. Temperature, pressure and the stability of competing phases are among the many factors that determine whether a material can be made or will exhibit favorable properties under the required operating conditions. Our research focuses on the use of first principles-based methods to predict synthesizable, enhanced materials that remain active under device relevant conditions. In this presentation, I will introduce our three-pronged approach which emphasizes synergies between (i) high throughput electronic structure calculations, (ii) phenomenological/empirical models for examining phase stability and (iii) experimental validation. As an example, I will present our recent work which explores Pb-free piezoelectrics and multiferroics. Here, I will discuss our efforts to map out the phase diagram of a Bi based oxide solid solution in order to identify a morphotropic phase boundary and our systematic examination of the strain-driven evolution of weak ferromagnetism in BiFeO₃. Together, these examples illustrate a framework for accelerating the design and experimental realization of novel functional materials. Research sponsored by the US DOE, Office of Science, BES, MSED using resources at NERSC.

11:15 AM

(EMA-S4-004-2017) Engineering organic solar cells with high performance computing (Invited)

E. Jankowski^{*1}; 1. Boise State University, USA

In order to meet projected global energy demands over the next 25 years, the equivalent of building a 2 GW coal power plant every few days is needed. Existing clean power generation technologies can meet this demand in principle, but their large short-term costs (relative to fossil fuels) limit their widespread adoption. In this work we aim to enable manufacturing of organic solar panels that pay for themselves in a few days by optimizing the structure of the organic active layer responsible for generating electricity. We perform coarse-grained molecular dynamics simulations accelerated with graphics processing units to determine the thermodynamically stable morphologies for a variety of candidate ingredients. Using these simulations we explain how morphology can be controlled using molecular self-assembly, identify promising candidate ingredients, and predict charge mobilities by incorporating semiempirical quantum chemistry calculations with device-scale morphologies.

11:45 AM

(EMA-S4-005-2017) Modeling of Soft Phonon Mode Dynamics and Phase Transitions in Aurivillius Type Ferroelectrics

S. K. Nayak^{*1}; F. Sun²; D. Maurya³; D. George⁴; A. Pramanick⁵; M. Kang³; H. Song³; A. Charkhesht⁴; G. Khodaparast⁴; N. Q. Vinh⁴; S. Priya³; P. S. Alpay²; 1. University of Connecticut, USA; 2. University of Connecticut, USA; 3. Virginia Tech, USA; 4. Virginia Tech, USA; 5. City University of Hong Kong, Hong Kong

The ferroelectric Bi₄Ti₃O₁₂ (BiT) compound belongs to the Aurivillius class with alternating layers of perovskite-like and anti-fluorite-like ionic arrangements in the crystal structure. The lattice constant (a,b,c) of the low temperature ferroelectric (monoclinic) phase is related to (a',a',c) of the high temperature paraelectric (tetragonal) phase as, a' = a/√2. Using THz spectroscopy and density functional theory (DFT) together with Phonopy we have studied the soft phonon modes for highly textured BiT films. Three low-frequency optical phonons were observed at room temperature with frequencies 0.61 THz, 0.83 THz and 0.95 THz. The DFT calculations predict the optical phonons with 1.13 THz, 1.14 THz, and 1.37 THz. The three low-frequency phonons shifted by 7.1%, 2.6% and 1.3%, respectively as temperature increased from -273 to 527°C. The corresponding displacement of phonon frequencies for 1% hydrostatic expansion of the lattice is found to be 12.9%, 5.3% and 2.6%, implying that phonon softening is associated with the volume expansion of the lattice. The majority contribution to the phonon density of states is from the heavier Bi atoms. The phonon modes suggest that the motion of atoms within the perovskite and anti-fluorite blocks are out-of-phase with respect to each other. The amplitude of displacement of Bi atoms in anti-fluorite layers is larger than in the perovskite layers.

12:00 PM

(EMA-S4-006-2017) Design of Functional Oxides using Machine Learning and Density Functional Theory

P. Balachandran^{*1}; J. Young²; J. Rondinelli³; T. Lookman¹; 1. Los Alamos National Lab, USA; 2. Drexel University, USA; 3. Northwestern University, USA

Many technological applications, including sensors and energy harvesters, make use of symmetry-dependent properties of intrinsically noncentrosymmetric (NCS) materials that lack the spatial inversion symmetry. However, NCS materials are challenging to discover because of the complex interplay between structure and chemistry. Here, we demonstrate a novel approach built on the foundations of applied group theory, machine learning and density functional theory to uncover quantitative symmetry-chemistry guidelines for the computational design of new NCS materials in the family of n=1 layered Ruddlesden-Popper oxides.

12:15 PM

(EMA-S4-007-2017) Electron anions control glass transition temperature in non-reducible oxidesL. Johnson¹; Y. Tomoda²; H. Hosono²; P. Sushko^{*1}; 1. Pacific Northwest National Lab, USA; 2. Tokyo Institute of Technology, Japan

Glasses are typically designed using different concentrations of network-forming (strongly bonded) and network-modifying (weakly bonded or chain-terminating) species, affecting properties such as glass transition temperature. In contrast, in a glass formed from the electride phase of cement $12\text{CaO} \times 7\text{Al}_2\text{O}_3$ (C12A7) known as mayenite, thermal and electronic properties are modified by replacing a small fraction of oxide ions with electrons. The resultant glass has composition $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32} \times (2e^-)$, where the electron anions act as solid-state analogue to solvated electrons. This material is a semiconductor with the workfunction of ~ 3.1 eV; its glass transition temperature is $\sim 160^\circ\text{C}$ lower than that in the parent oxide, yet no detectable structural changes was observed. Ab initio molecular dynamics simulations reveal the glass formation process in C12A7 and elucidate structural and electronic changes in the stoichiometric and electride forms of material; we found that electron anions function as network modifiers, replacing oxide ions and forming highly mobile network links. We propose that electron anions present a new control parameter for glasses formed from non-reducible oxides and that the rate of movement of weak links through a network, even at low concentrations, may be crucial for understanding disordered systems. LE Johnson, PV Sushko, Y Tomota, H Hosono, Proc Natl Acad Sci USA 113, 10007 (2016)

S5: Energy Sustainable Optoelectronics and Magnetoelectronics**Low-Dimensional Electronic Materials for Energy and Logic**

Room: Mediterranean C

Session Chair: Jian Shi, Rensselaer Polytechnic Institute

10:00 AM

(EMA-S5-015-2017) Adaptive, programmable oxide electronics for energy efficient devices (Invited)S. Ramanathan^{*1}; 1. Purdue University, USA

Convergence in computing, communications and internet of things are driving the search for new semiconductors that can usher in an era of low voltage, steep slope, low power dissipating solid state devices. One class of materials that are particularly promising to explore in this regard are oxides that can change phase under external stimuli, show multiple stable resistance states or simply demonstrate reversible soft breakdown characteristics under strong electric fields. In this presentation, I will consider disordered oxides that can be switched in a non-volatile manner and contrast them with Mott insulators where electronic phases can be crossed with and without lattice symmetry changes. These systems pose several puzzles that require cross-disciplinary collaborative studies involving dynamical measurements, first principles modeling and the microscopic connection between disorder and emergent states. A few examples from our laboratory on rutile and perovskite oxides will be discussed and will be placed in the context of broader efforts in the field to both understand many body effects in real materials and the use of solid state device response to establish underlying physical mechanisms. Time permitting, I will also present a brief comparison to chalcogenides that possess a sub-set of these fascinating properties.

10:30 AM

(EMA-S5-016-2017) Graded Nanowire Interfaces for Efficient Energy Conversion (Invited)M. H. Malakooti¹; H. A. Sodano^{*2}; 1. University of Michigan, USA; 2. University of Michigan, USA

Vertically aligned nanowires can be used to design graded interfaces between two dissimilar phases. This material blend at the interface region may lead to novel products with controlled material properties for desired applications. One of these applications can be energy conversion at the interface, where a considerable amount of mechanical load transfers. In this paper, through a hydrothermal reaction vertically aligned lead zirconate titanate (PZT) nanowires are directly grown on a PZT thin film. The optimized synthesis parameters resulted in growth of nanowires with an average length of 10 microns and average diameter of 100 nanometers. To demonstrate the electromechanical properties of these nanowire interface, miniature energy harvesting devices are fabricated. In these devices, PZT film is coated on a thick titanium foil as the bottom electrode and followed by the hydrothermal reaction for the synthesis of vertically aligned PZT nanowires. After adding the top electrode on the nanowires and packaging the device in an epoxy matrix, vibration tests are conducted to study the ability of these nanowire interfaces in power generation. Measured voltage and current show the feasibility of the stable energy harvesting using the fabricated beam composed of nanostructured PZT phase. This result indicates the great potential of the synthesized nanowire arrays for energy conversion at nanoscale.

11:00 AM

(EMA-S5-017-2017) Piezotronics-Regulated Electrochemical and Catalytic Materials and Devices (Invited)X. Wang^{*1}; 1. University of Wisconsin, USA

Recent discovery of the piezotronic effect revealed that when a strain is experienced by a piezoelectric semiconductor material or device, it can introduce interfacial charge redistribution and lead to significant performance gain or new functionality. Three piezotronic-enhanced or enabled applications will be introduced as successful examples. The piezotronic effect has been applied to the ZnO/PbS quantum dot heterojunction for engineering the interfacial band structure and depletion region and escalated the solar energy efficiency. Similarly, piezotronic effect could enhance the oxygen evolution reaction (OER) in photoelectrochemical (PEC) systems in a $\text{Ni}(\text{OH})_2$ -decorated ZnO photoanode system by physically deflecting the photoanode. A largely enhanced performance of PEC photoanodes was also obtained by ferroelectric polarization-endowed band engineering on the basis of $\text{TiO}_2/\text{BaTiO}_3$ core/shell nanowires. Numerical model was established to calculate the potential distribution across the catalyst/piezoelectric/electrolyte heterojunction and reveal favorable electronic band bending as a result of internal piezoelectric polarization. In summary, interfacing between piezotronics and electrochemical systems will open a new route for engineering the catalytic properties of conventional catalysts via mechanical straining.

11:30 AM

(EMA-S5-018-2017) Scalable 3-D Nanostructure Array Integration and Manufacturing: A Nanomaterials Roadmap toward Ultrahigh Efficiency, Robustness, and Multi-functionality (Invited)P. Gao^{*1}; 1. University of Connecticut, USA

Three-dimensional (3-D) integration of nanostructures or nanostructure arrays into applicable platforms or devices represents the need for meeting ever-increasing demands of human beings for cost-effectiveness, structure sophistication, multi-function enabling, while simplified and efficient practical operations. Such an integration process generally involves a diverse array of nanostructured entities that include various dissimilar nanoscale building blocks

such as nanoparticles, nanowires, and nanofilms made of metals, ceramics, or polymers in the nanoscale form. In this talk, I will highlight our latest research progress on the 2-D and 3-D metal oxide and metal based nanostructure integrations toward applicable ultrahigh efficiency, robustness, and improved functionality, with an intention to draw a unique roadmap toward practically and better bridging the gap between nanoscience and nanotechnology in energy and environmental applications. Specifically, examples through design in scalable nanomanufacturing, catalytic exhaust aftertreatment, chemical and physical sensing will be used as the connecting dots to display the nanomaterials roadmap linking from scalable 2-D toward 3-D integration.

12:00 PM

(EMA-S5-019-2017) Piezotronics in 2D materials (Invited)

W. Wu^{*1}; 1. Purdue University, USA

Monolayer transition metal dichalcogenide (TMDCs) have been theoretically predicted to exhibit piezoelectricity due to the strain induced lattice distortion and associated ion charge polarization, suggesting possible applications of these 2D nanomaterials in nano-scale electromechanical devices that take advantage of their outstanding semiconducting and mechanical properties. Recently, the first experimental observation of piezoelectricity in single atomic layer 2D MoS₂ and its application in mechanical energy harvesting and piezotronic sensing was demonstrated. Cyclic stretching and releasing of odd-layer MoS₂ flakes produces oscillating electrical outputs, which converts mechanical energy into electricity. More significantly, transport measurements show a strong piezotronic effect in single-layer MoS₂, but not in bilayer and bulk MoS₂. The coupling between piezoelectricity and semiconducting properties in a broad range of two-dimensional nanomaterials may enable the development of applications in powering nanodevices, adaptive bioprobes and tunable/stretchable electronics/optoelectronics.

S9: Interfaces in Microstructural Evolution: Structure, Properties, Anisotropy, and Motion

Atomistics of Microstructure Evolution

Room: Mediterranean A/B

Session Chairs: Wayne Kaplan, Technion - Israel Institute of Technology; Wolfgang Rheinheimer, Karlsruhe Institute of Technology

10:00 AM

(EMA-S9-015-2017) Interfacial step alignment as a new mechanism of hetero-epitaxy/orientation relationships (Invited)

D. Chatain^{*1}; P. Wynblatt²; A. Rollett²; G. Rohrer²; 1. Aix Marseille Univ. - CNRS, France; 2. Carnegie Mellon University, USA

How and why do two fcc materials, of very different lattice parameters, choose their relative orientations across their hetero-interface? To answer this question, the orientation relationships (ORs) of submicron Ag crystals equilibrated on more than 200 Ni(hkl) surfaces, spanning the whole stereographic triangle, have been determined by EBSD. The observed ORs do not conform entirely to either of the common beliefs: (i) that Ag will form with its (111) plane parallel to any Ni(hkl) surface, or (ii) that the OR between Ag and Ni will be cube-on-cube. Although the cube-on-cube OR is indeed observed, three other types of OR have been identified. The experimental results are consistent with MD simulations, which show that the ORs are related to the step alignment which develops in the early stages of interface formation and which leads to minimum energy interfaces. This is a new concept for the interpretation of hetero-epitaxy and/or ORs.

10:30 AM

(EMA-S9-016-2017) A Microstructural Study of Bilayer Graphene Using Phase Field Crystal Simulations (Invited)

R. V. Zucker^{*1}; M. Asta¹; 1. University of California, Berkeley, USA

Controlling partial dislocations in multilayer graphene has the potential to enhance electronic properties. However, little is known about the stability of a given arrangement of dislocations, how dislocations interact, and their anisotropy. We use structural phase field crystal (PFC) simulations, which can simultaneously provide atomic-scale resolution of defects and micron-scale resolution of microstructure, to study dislocation dynamics in bilayer graphene. The PFC simulations were coordinated with atomistic simulations and experiments to ensure that the simulations are realistic. Strong anisotropy and high dislocation mobilities lead to a surprisingly rich variety of behaviors. Knowledge of microstructural behavior in bilayer graphene can be used to identify stable defect structures whose electronic properties may be exploited in future device designs.

11:00 AM

(EMA-S9-017-2017) Alumina Reinforced with Continuous Fibers of Carbon Nanotubes: Interface Characterization and Mechanical Properties

R. Marder^{*1}; W. D. Kaplan¹; 1. Technion - Israel Institute of Technology, Israel

The nature of the interface between matrix and reinforcing phases in composites is critical in defining electronic and/or mechanical properties. The introduction of carbon nanotubes (CNTs) as a reinforcing phase for a ceramic matrix is interesting as it is expected to produce a composite with improved fracture toughness. However, achieving a homogeneous dispersion of CNTs with strong bonding between nanotubes and the matrix is challenging. In the current research alumina based composites were produced with continuous mats of CNTs. The use of continuous CNT mats is advantageous, as it offers the possibility to overcome deflocculation problems. Composites were sintered to full density (98%) at 1600°C for 2 h in a graphite furnace using a He atmosphere, to protect the CNTs from oxidation. The alumina-CNT interface morphology was characterized by electron microscopy. Cr was added as a dopant to improve alumina-CNT adhesion. The role of Cr as dopant will be discussed. The flexural strength of the composites was measured and compared to monolithic alumina. It was found that the presence of carbon during sintering had a positive effect on the mechanical properties of alumina.

11:15 AM

(EMA-S9-018-2017) Low-angle tilt grain boundaries in SrTiO₃ (Invited)

R. A. De Souza^{*1}; 1. RWTH Aachen University, Germany

There is renewed interest in the atomistic structure and transport properties of dislocations in the perovskite oxide SrTiO₃, driven by the material's possible application in devices for all-oxide electronics and resistive switching. Low-angle grain boundary constitute elegant systems for studying dislocations. In my talk, I will briefly introduce, first, the bulk defect chemistry of acceptor-doped SrTiO₃, and then, the thermodynamics of space-charge formation at extended defects. The main part of the talk will concentrate on understanding the structure and properties of low-angle tilt bicrystals of this prototypical perovskite-type oxide. In particular I will focus on the behavior as a function of misorientation angle, and I will emphasise the benefits of combining experimental and computational approaches.

11:45 AM

(EMA-S9-019-2017) Disconnections at general grain boundaries in SrTiO₃ and their role in grain boundary motion (Invited)

H. Sternlicht^{*1}; W. Rheinheimer²; A. Mehlmann¹; A. Rothchild¹;
M. J. Hoffmann²; W. D. Kaplan¹; 1. Technion, Israel; 2. Karlsruhe Institute of Technology, Germany

The kinetics of grain boundary (GB) motion can be determined experimentally by measuring the average grain size in samples annealed at different temperatures for different durations. In SrTiO₃ annealed under an oxidizing atmosphere, the GB mobility was previously found to decrease with an increase in temperature (in the temperature range of 1350-1425°C), deviating from the expected Arrhenius behavior. While GB mobility can be measured, the mechanism by which a GB moves has not yet been determined at the atomistic level in general polycrystalline systems. The present work focuses on the atomistic mechanism by which GBs migrate, using high resolution transmission electron microscopy (HRTEM) and SrTiO₃ as a model system. In this work, general GBs in SrTiO₃ annealed under an oxidizing atmosphere are studied ex-situ, and compared to the surface of SrTiO₃ grains which are studied in-situ under vacuum. The appearance of steps and ledges in both in-situ and ex-situ experiments in SrTiO₃ annealed under an oxidizing atmosphere indicate their role in the GB motion process. In addition, GBs in samples annealed in reducing atmosphere will be discussed in light of the results from annealing under oxidizing atmosphere. Such samples were previously shown to accommodate wetting films at many boundaries.

12:15 PM

(EMA-S9-020-2017) Towards a Predictive Model for Grain Boundary Dynamics (Invited)

J. Han^{*1}; V. Vitek¹; D. Srolovitz¹; 1. University of Pennsylvania, USA

A useful picture of grain boundary (GB) dynamics should explain such phenomena as GB migration, GB shear coupling, GB sliding and GB roughening. These phenomena are, in turn, controlled by GB disconnections, which are linear defects characterized by a dislocation Burger vector and a step height. In this presentation, we first enumerate the disconnections that are permitted by the GB bicrystallography. Then, we present a simple model for disconnection energetics and use it to develop a statistical mechanics description of GB dynamics. We apply this model to predict shear coupling as a function of GB geometry. Next, we consider how GBs roughen with increasing temperature. We then use this approach to explain the transition from GB shear coupling to GB sliding. Finally, we examine how these GB-geometry- and temperature-dependent disconnection dynamics control GB migration and microstructure evolution. This approach leads to a much more quantitative understanding of GB properties than current theories.

S10: Interfacial Phenomena in Multifunctional Heterostructures: From Theory to Transport Processes**Micro/Nanoscale Theoretical and Experimental Studies of Interfacial Phenomena**

Room: Caribbean B

Session Chair: Anderson Janotti, University of Delaware

10:00 AM

(EMA-S10-001-2017) Defects, band alignment and electron charge redistribution in NdTiO₃/SrTiO₃ heterostructures (Invited)

P. Sushko^{*2}; P. Xu⁴; T. Droubay²; Y. Ayino⁴; C. Cheng⁴; V. S. Pribiag⁴;
J. Jeong⁴; K. Mkhoyan⁴; R. Comes¹; B. Jalan⁴; S. Chambers³; 1. Auburn University, USA; 2. Pacific Northwest National Lab, USA; 3. Pacific Northwest National Laboratory, USA; 4. University of Minnesota, USA

A recent study demonstrated that SrTiO₃/NdTiO₃/SrTiO₃ (STO/NTO/STO) heterostructures give rise to a high-density, two-dimensional electron gas (2DEG) in the STO exceeding $3 \times 10^{15} \text{ cm}^{-2}$. Here we examine approaches to controlled manipulation of the 2DEG density by judicious selection of the width of the NTO layer and the concentrations of cation vacancies and oxygen interstitials. Ab initio simulations based on density functional theory show that at low NTO thickness (t), STO/NTO/STO becomes metallic for $t=2$ u.c. due to electronic reconstruction in which Ti at interfacial TiO₂ planes acquire an average charge of 3.5+ and the 2DEG density is $\sim 3 \times 10^{14} \text{ cm}^{-2}$ per interface. As t increases, the NTO lower Hubbard band, which is degenerate with the bottom of the STO conduction band, becomes wider and passes additional electrons to the 2DEG. In contrast, NTO/STO heterostructures without an STO cap show no measurable conductivity for $t < 4$ u.c, which points to surface modification due to air exposure. Calculated formation energies of interstitial oxygen defects in NTO suggest that NTO can readily adsorb oxygen and, accordingly, convert Ti³⁺ to Ti⁴⁺. This result indicates that surface reactivity can be exploited to control the insulator-to-metal transition in this system. P. Xu, et. al., Adv. Mater. Interfaces 3, 1500432 (2015); Phys. Rev. Lett. 117, 106803 (2016).

10:30 AM

(EMA-S10-002-2017) Extracting buried electronic and magnetic structure information from oxide heterostructures with resonant x-ray spectroscopy (Invited)

R. Green^{*1}; G. Sawatzky¹; 1. University of British Columbia, Canada

In this talk, I will present some of our recent work using different forms of resonant soft x-ray spectroscopy to uncover key properties in several oxide heterostructure systems. Using resonant x-ray reflectometry, we are able to determine depth-dependent orbital occupations in oxide heterostructures, allowing the quantification of electronic and orbital reconstructions. We have applied this to the highly studied LaAlO₃/SrTiO₃ system, as well as STO-based 2DEG systems which utilize manganite buffer layers to enhance electron mobilities. Using resonant x-ray diffraction, we have probed in detail the magnetic order in nickelate heterostructures. Not only do we find magnetic structures in agreement with recent bond disproportionation theories, but we also find that the magnetic order can be tuned by varying the dimensionality of 111-oriented NdNiO₃ films embedded in NdGaO₃ matrices. I will give an overview of these findings while highlighting the recent developments in resonant x-ray spectroscopy which show it to be an ideal tool for the study of oxide heterostructures.

11:00 AM

(EMA-S10-003-2017) Oxygen transport phenomena at the grain boundary level in MIEC thin films (Invited)

F. Chiabrera¹; A. Saranya¹; D. Pla¹; A. Morata¹; A. Cavallaro²; J. Canales-Vazquez³; J. Kilner²; M. Burriel⁴; A. Tarancón⁴; 1. IREC, Spain; 2. Imperial College, United Kingdom; 3. UCLM, Spain; 4. Grenoble-INP, France

Nanoionics has become an increasingly promising field for the future development of advanced energy conversion and storage devices, such as batteries, fuel cells, and supercapacitors. Particularly, nanostructured materials offer unique properties or combinations of properties as electrodes and electrolytes in a range of energy devices. However, the enhancement of the mass transport properties at the nanoscale has often been found to be difficult to implement in nanostructures. In this talk, we will detail the fabrication of an artificial mixed ionic electronic conducting oxide obtained by grain boundary (GB) engineering thin films of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3+\delta}$. This electronic conductor is converted into a good mixed ionic electronic conductor by synthesizing a nanostructure with high density of vertically aligned GBs with high concentration of strain-induced defects. Since this type of GBs present a remarkable enhancement of their oxide ion mass transport properties (of up to six orders of magnitude at 773 K), it is possible to tailor the electrical nature of the whole material by nanoengineering, especially at low temperatures. The results of this study leads to fundamental insights into oxygen diffusion along GBs and to the application of these engineered nanomaterials in new advanced solid state ionics devices such as micro-solid oxide fuel cells or resistive switching memories.

11:30 AM

(EMA-S10-004-2017) A New Line Defect in NdTiO_3 Perovskite (Invited)

J. Jeong²; M. Topsakal²; P. Xu²; B. Jalan¹; R. Wentzcovitch²; K. Mkhoyan²; 1. University of Minnesota, USA; 2. University of Minnesota, USA

Perovskite oxides form an eclectic class of materials owing to their structural flexibility in accommodating cations of different sizes and valences. They host well known point and planar defects, but so far no line defect has been identified other than dislocations. Using analytical scanning transmission electron microscopy (STEM) and ab initio calculations we have detected and characterized the atomic and electronic structures of a novel line defect in NdTiO_3 perovskite. It appears in STEM images as a perovskite cell rotated by 45 degrees. It consists of self-organized Ti-O vacancy lines replaced by Nd columns surrounding a central Ti-O octahedral chain containing Ti^{4+} ions, as opposed to Ti^{3+} in the host. The distinct Ti valence in this line defect introduces the possibility of engineering exotic conducting properties in a single preferred direction and tailoring novel desirable functionalities in this Mott insulator.

12:00 PM

(EMA-S10-005-2017) Realistic Atomistic Modeling of Surfaces and Interfaces

A. Blom¹; U. M. Pozzoni¹; K. Stokbro¹; 1. QuantumWise, Denmark

The understanding of interfaces at the microscopic level is still very limited, since direct observations of its electronic properties are impossible. Interfaces (and surfaces) also constitute a challenge for simulations, since standard atomic-scale approaches are limited to periodic, undoped systems in equilibrium, and continuum models cannot capture the detailed interface chemistry. We will present an efficient atomistic simulation approach to resolve these issues. Utilizing non-equilibrium Green's function (NEGF) techniques in combination with density-functional theory (DFT), it is possible to correctly describe not only single interfaces, but also free surfaces. The method can be applied to metal (M)/semiconductor (S) interfaces, as well as S/S or M/M ones, e.g. between different materials or grain orientations. It can also be applied to ultrathin layers embedded between bulk materials. A finite bias can

be applied, making it possible to compute I-V curves and Schottky barriers, naturally taking into account both thermionic emission and tunneling, and effects like semiconductor doping, impurities, vacancies, etc. Several examples in systems relevant for solar cells, semiconductors, batteries, catalysis, and other applications areas, will be shown, and the results will be compared with approaches typically used in the literature, which will be shown to not only often be wrong, but also more computationally demanding.

12:15 PM

(EMA-S10-006-2017) Excitons at oxide interfaces in ellipsometric spectra

S. Zollner¹; C. Rodriguez¹; N. Samarasingha¹; J. Moya¹; N. Fernando¹; P. Ponath²; K. Kormondy²; A. Demkov²; S. Chattopadhyay³; 1. New Mexico State University, USA; 2. University of Texas, USA; 3. Indian Institute of Technology, India

Excitonic features in optical constants and ellipsometry spectra of semiconductors and insulators have been studied for many years. An exciton is an electron-hole pair bound by the Coulomb interaction, with properties similar to a H atom. In an epitaxial layer on a substrate with a different band gap, the wave functions of electron and hole are strongly modified. In a type-I quantum well, consisting of a narrow-gap semiconductor grown on a large-gap substrate, both electron and the hole are confined, which leads to an increase in the dipole overlap matrix element. Therefore, the dominant absorption peak at 4.2 eV is larger in a 20 nm thick SrTiO_3 layer on LaAlO_3 than in bulk SrTiO_3 . (The band gap of LaAlO_3 is larger than that of SrTiO_3 .) On the other hand, in a staggered type-II quantum well, either the electron is confined, or the hole, but not both. Therefore, the overlap dipole matrix element (and the excitonic absorption) is strongly reduced, because one quasiparticle resides in the quantum well and the other in the substrate. If a SrTiO_3 layer is grown on Si or Ge, the valence band maximum occurs in the substrate, while the conduction band offset is very small. Therefore, the exciton wave function is delocalized, which reduces the dipole overlap matrix element. Therefore, the real and imaginary part of thin SrTiO_3 layers on Si or Ge are much smaller than in the bulk and decrease monotonically with decreasing thickness.

S14: Multifunctional Nanocomposites

Multifunctional Nanocomposites: Functionality by Design II

Room: Caribbean C

Session Chair: Ho Nyung Lee, Oak Ridge National Laboratory

10:00 AM

(EMA-S14-015-2017) Flexible Multiferroic Nanocomposite with Ultra-High Magnetoelectric Coupling (Invited)

Y. Chu¹; 1. National Chiao Tung University, Taiwan

Nowadays, the flexible devices have attracted lots of attentions due to their potential to change our daily life. However, to explore more possibilities in flexible devices, additional degrees of freedom are highly on demand. Flexible memory is one such attribute which has attracted long-standing attention in today's energy-conscious world as it is the fundamental component of modern electronics. In order to develop a new non-volatile memory device, the use of magnetoelectric multiferroics has been proposed with combined advantages of ferroelectric and magnetic memories to deliver a low-energy consumption memory device. In this presentation, we investigate the magnetoelectric coupling in self-assembled vertically aligned BFO-CFO nanocomposites wherein BFO nanopillars embedded in CFO matrix exhibit an incoherent growth on mica with minimal substrate clamping. The magnetic and electrical measurements highlight the enhanced magnetoelectric coupling between BFO-CFO desirable for highly sensitive magnetic sensor application. Moreover,

the fabricated nanocomposite also offers the additional advantage of being flexible. Therefore, this study provides a platform for fabricating highly-sensitive and flexible magnetoelectric sensors that are robust against extreme conditions with optimized performance.

10:30 AM

(EMA-S14-016-2017) Novel perpendicular exchange bias in vertical aligned nanocomposite films through interfacial coupling

M. Fan^{*1}; W. Zhang¹; J. Jian²; J. Huang²; H. Wang²; 1. Texas A&M University, USA; 2. Purdue University, USA

Exchange bias in the out-of-plan direction is of great interest for its potential applications in advanced spintronic devices. In this talk we report that, via confining the ferromagnetic (FM) / anti-ferromagnetic (AFM) heterointerfaces in the vertical direction, epitaxial vertically aligned nanocomposite (VAN) films provide a powerful platform to enable strong perpendicular exchange bias effects (PEB). $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$: LaFeO_3 nanocomposite thin films have been deposited on SrTiO_3 (001) substrates by pulsed laser deposition (PLD). X-ray diffraction (XRD) and transmission electron microscopy (TEM) results show distinguished epitaxial columnar in matrix structures with systematical strain tuning effect. Remarkable exchange bias effects have been detected in the nanocomposite films and could be modulated with composition variation as well as different cooling field. Detailed discussion suggests the vertical interface coupling associated with a disordered spin-glass state plays an important role in such EB efforts.

10:45 AM

(EMA-S14-017-2017) Tuning functionalities in nanocomposite metal-oxide films by strain engineering (Invited)

A. Chen¹; J. Hu²; E. Enriquez³; P. Lu⁴; H. Wang⁵; L. Chen⁶; J. MacManus-Driscoll⁷; M. Fitzsimmons⁸; Q. Jia^{*9}; 1. Los Alamos National Lab, USA; 2. University of Wisconsin, USA; 3. Los Alamos National Lab, USA; 4. Sandia National Laboratories, USA; 5. Purdue University, USA; 6. Pennsylvania State University, USA; 7. University of Cambridge, United Kingdom; 8. Oak Ridge National Laboratory, USA; 9. University at Buffalo, USA

Thin films, coatings, and nanostructured materials have found extensive applications in virtually all technological and scientific areas. Challenges, however, remain in controlled synthesis of epitaxial films with desired compositional and structural attributes which are the key parameters in determining the properties and functionalities in the real materials systems. In this talk, I will discuss our approaches to the management of lattice strains to tune the functionalities of a range of functional materials. Specifically, I will use epitaxial nanocomposite ferroic films as model systems to illustrate the effect of strain on the functionalities of metal-oxide films.

11:15 AM

(EMA-S14-018-2017) Enhanced Tunable Magnetic and Transport Properties in Epitaxial $(\text{Pr}_{0.5}\text{Ba}_{0.5}\text{MnO}_3)_{1-x}(\text{CeO}_2)_x$ Nanocomposite Thin Films

L. Shen^{*1}; C. Ma²; S. Cheng¹; S. Ren¹; S. Cheng¹; S. Mi¹; M. Liu¹; 1. Xi'an Jiaotong University, School of Electronic and Information Engineering, China; 2. Xi'an Jiaotong University, State Key Laboratory for Mechanical Behaviour of Materials, China

Epitaxial self-assembled vertically aligned nanocomposite (VAN) $(\text{Pr}_{0.5}\text{Ba}_{0.5}\text{MnO}_3)_{1-x}(\text{CeO}_2)_x$ (PBMO:CeO₂) and pure PBMO films were fabricated on (001) (La,Sr)(Al,Ta)O₃ substrates by pulsed laser deposition. By modulating the molar ratio of CeO₂ phase ($x=0.1, 0.2, 0.35, 0.5, 0.7$), tunable transport properties over a wide temperature range as well as low-temperature magnetization are demonstrated in the nanocomposite thin films. Besides confirmation of the in-plane and out-of-plane orientation using X-ray diffraction, transmission electron microscopy study has revealed columnar structure of PBMO:CeO₂ ($x=0.5$) with column width around 10~20 nm and distinct phase separation between PBMO and

CeO₂ from energy dispersive X-ray spectroscopy measurement. Compared with the pure PBMO thin film, the vertical compressive strain induced by CeO₂ partially relaxes the in-plane and out-of-plane strain of PBMO, and the magnetization of the VAN thin film ($x=0.5$) is enhanced and almost two times higher than the pure film. Moreover, the relaxed strain and the insulating CeO₂ nanopillars acting as the energy barrier induce the larger resistivity and enhanced magnetoresistance. All of these phenomena indicate that the VAN structure is an effective method to tune the strain states in thin film and obtain desired physical properties.

11:30 AM

(EMA-S14-019-2017) Engineering the ferroic orders at $\text{BiFeO}_3/\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ interfaces (Invited)

E. Guo^{*1}; 1. Oak Ridge National Lab, USA

Artificially engineered epitaxial heterostructures enable new functionalities that cannot be realized from the individual constituents. Utilizing the external stimulations, like strain and electrostatic doping, gives a good handle to investigate the ferroelectric switching and ferromagnetic order in multiferroic hybrids. In this talk, firstly, I will show the ferroelectric switching dynamics of BiFeO_3 (BFO) capacitors can be effectively controlled by applying in-situ reversible controlled strain through a piezoelectric substrate. The domain dynamics under different strain states are studied using a piezo-response force microscopy. The velocity of domain walls can be reversibly changed by more than one order of magnitude through ~0.1% in-plane strain. The strain controlled depolarization charges on the domain walls and different ferroelastic switching paths are suggested mechanism that dominant the complex switching dynamics. In the second part of the talk, I will report a ferromagnetic state is observed in ultrathin BFO layers, sandwiched between manganite layers. While the BFO ultrathin layers maintain a good ferroelectric property, both polarized neutron reflectometry and x-ray magnetic circular dichroism reveal that the spin state of BFO is anti-parallel to the magnetization of LSMO. We attribute the novel ferromagnetic state of BFO is related to the electronic orbital reconstruction at the interfaces.

11:45 AM

(EMA-S14-020-2017) Nanoscale manipulations of the structural and electronic phases of vanadium oxides (Invited)

D. Schrecongost¹; M. Aziziha¹; W. Dai¹; H. Zhang²; R. Engel-Herbert³; C. Cen^{*1}; 1. West Virginia University, USA; 2. Pennsylvania State University, USA; 3. Pennsylvania State University, USA

The capability of generating sharp material contrasts in small length scales is the major enabler of high performance electronic and photonic devices. Here we show that the transitions between three distinct VO₂ based material phases can be controlled in nanoscale by conducting atomic force microscope (c-AFM). Such result was achieved by field ionization of the spontaneously formed water meniscus at probe-sample junction and the resultant localized ion reactions with VO₂. The three phases, including two close-packed structures with monoclinic/rutile-like lattices and a layered structure with Van der Waals interlayer coupling, differ not only structurally but also in their metallicity and optical properties. Using the c-AFM writing technique, arbitrary nano-patterns of the three phases as well as their in-plane heterostructures can be deterministically created, which is highly useful for producing advanced multifunctional device architectures on demand.

12:15 PM

(EMA-S14-021-2017) Ultrahigh Energy Storage Performance of Lead-Free Oxide Multilayer Film Capacitors via Interface Engineering

M. Liu^{*1}; Z. Sun³; C. Ma²; H. Wang³; C. Jia⁴; 1. Xi'an Jiaotong University, China; 2. Xi'an Jiaotong University, China; 3. Xi'an Jiaotong University, China; 4. Xi'an Jiaotong University, China

Ultrahigh energy storage density of 52.4 J/cm³ with great efficiency of 72.3% has been achieved at room temperature by interface engineering of epitaxial multilayers based on environment-friendly BaTiO₃-based dielectrics. The electric breakdown strength and thus energy storage density are significantly improved by increasing the number of interfaces in the multilayer systems, which effectively impede the spread and growth of the electric trees, revealed by numerical simulations based on finite element method. Most importantly, the multilayer systems exhibit excellent thermal stability with energy density of ~ 34.8 J/cm³ and efficiency of ~ 75.1% over wide temperature range from RT to 140°C, which are the highest values obtained up to now in the lead-free material systems and comparable to the best energy storage performance reported for the lead-based systems. Our results demonstrate that interface engineering is an effective way in tuning/improving the energy storage performances in the BaTiO₃-based multilayer systems. The outstanding performances of energy storage provide solid basis for widespread applications of the thin film systems in modern electronic and power modules in harsh working environments.

S15: Superconducting Materials and Applications

Issues Related to the Fabrication of Low-cost and High-performance Second Generation Coated Conductors

Room: Pacific

Session Chairs: Haiyan Wang, Purdue University; Charles Rong, U.S. Army Research Laboratory

10:00 AM

(EMA-S15-013-2017) Current-Limiting Mechanisms in Superconductors at High Temperatures and Magnetic Fields (Invited)

A. Gurevich^{*1}; 1. Old Dominion University, USA

Since the discoveries of high-T_c cuprates and ferropnictides the quest for new superconductors has shifted toward more anisotropic, strongly correlated materials with lower carrier densities and competing antiferromagnetic orders. While these features enhance superconducting correlations, they also result in such serious problems for applications, that the high critical temperature T_c and the upper critical field are no longer the main parameters of merit. Instead, the current-carrying capability of cuprates and Fe-based superconductors at high fields and temperatures becomes mostly limited by thermally-activated hopping of vortices and electromagnetic granularity. This talk gives an overview of current-limiting mechanisms and limits of critical current densities which could be achieved by optimizing pinning defect nanostructure. I will also discuss physical and material restrictions to be satisfied in order to make superconductors useful at high temperatures and magnetic fields. These restrictions become essential at higher temperatures and magnetic fields, particularly for the yet-to-be-discovered room temperature superconductors if they will be used above 77K. In this case the ability of superconductors to carry non-dissipative currents would be mostly limited by fluctuations for which higher carrier density and weaker anisotropy are more essential than higher pairing temperature.

10:30 AM

(EMA-S15-014-2017) REBCO cable AC losses and transport performance limitations under mechanical bending (Invited)

A. Nijhuis^{*1}; 1. University of Twente, Netherlands

A detailed method of stress-strain state modeling in CORC conductors was developed. The model is based on Finite Element Method (FEM) and extensive strain measurements on REBCO tapes. Systematic measurements on single REBCO tapes were carried out combining axial tension and torsion as well as transverse loading. The FE model takes into account temperature dependence and the elastic-plastic properties of the tape materials and includes initial processing conditions during tape manufacture up to magnet operating conditions. Furthermore a comparison of FEM simulations with CORC cable bending experiments is presented with special attention for the critical bending radius as the threshold where the tapes in the CORC become irreversibly degraded. The influence of tape inter-layer friction was also investigated. In addition the AC loss of different HTS cable types were measured in alternating magnetic fields including Conductor On Round Core (CORC) cables, stacked tape conductors and Roebel cable. The applied AC magnetic field is sinusoidal with amplitudes in the range of 5 to 400 mT and frequencies up to 0.1 Hz. The AC loss of CORC and Roebel cable was measured at 4.2 and 77 K. Intertape contact resistance measurements showed that high tape-to-tape contact resistance severely limits current sharing between REBCO tapes in HTS cables. An brief overview of the results is presented.

11:00 AM

(EMA-S15-015-2017) Strain mediated self-assembly of strong and isotropic artificial pinning centers in YBCO nanocomposite films (Invited)

J. Wu^{*2}; S. Chen²; M. P. Sebastian¹; B. Gautam²; J. Shi²; T. J. Haugan¹; 1. AFRL, USA; 2. University of Kansas, USA

Generating strong and isotropic artificial pinning centers (APCs) is key to optimize pinning in superconducting YBCO thin films and coated conductors. Understanding the interplay of the relevant strain fields provides an effective approach of controllable self-assembly of APCs with desired morphology, orientation and dimension. In this work, we explore a few ways towards effective generation of strong and isotropic APCs from either single APC materials (such as BZO) or double APC materials (such as Y₂O₃ and BZO). Transport critical current density J_c(H, T, q) measured on these samples revealed strong and isotropic pinning landscape can be generated using both single doping as well as double doping. This resulted in a significantly enhanced pinning force density F_p(H) as well as almost no angular dependence on the magnetic field irritations. By fitting the Dew-Hughes equation of the pinning force density F_p(H) at orientations of H at 0 (H//c-axis), 45, and 90 deg (H//ab) we extract the scaling behaviors of the F_p(H) associated to the BZO-NRs and isotropic BZO and Y₂O₃ NPs. Additional analysis of the flux creep rate through the "N" value fitting provides insights in the pinning potentials associated to different types of APCs. This result sheds light on approaches towards interactive control of strong and isotropic APCs in YBCO films and coated conductors.

11:30 AM

(EMA-S15-016-2017) Study of the Flux Pinning Landscape of YBCO Thin Films with Single and Mixed Phase Additions BaMO₃ + Z: M=Hf, Sn, Zr and Z = Y₂O₃, Y₂11 (Invited)

M. P. Sebastian^{*1}; J. Reichart¹; M. Ratcliff²; T. Bullard²; J. Burke¹; C. B. Ebbing³; G. Panasyuk²; C. Tsai⁴; W. Zhang⁴; J. Huang⁴; H. Wang⁴; J. Wu⁵; T. J. Haugan¹; 1. AFRL, USA; 2. UES, USA; 3. UDRI, USA; 4. Texas A&M University, USA; 5. University of Kansas, USA

Addition of nanophase defects to YBa₂Cu₃O₇ (YBCO) superconductor thin films enhances flux pinning, and results in increasing current densities. While previous studies focused on single-phase additions such as BaSnO₃, BaZrO₃, and Y₂BaCuO₅ (Y₂11); the

addition of several phases has shown strong improvements by combining different flux pinning mechanisms. This paper explores the effect of mixed phase nanoparticle pinning, with the addition of insulating, nonreactive phases of: 1) $\text{BaSnO}_3 + \text{Y}_2\text{O}_3$, 2) $\text{BaSnO}_3 + \text{Y}_2\text{TiO}_5$, 3) $\text{BaZrO}_3 + \text{Y}_2\text{O}_3$, and 3) $\text{BaHfO}_3 + \text{Y}_2\text{O}_3$. Processing parameters vary the doped YBCO single target volume percent of either BaHfO_3 , BaSnO_3 , or BaZrO_3 , while maintaining either Y_2O_3 or Y_2TiO_5 constant at 3 vol. %. Pulsed laser deposition produces films on LaAlO_3 and SrTiO_3 substrates at deposition temperatures of 750–840°C. Current density is measured for fields ranging from $H = 0-9 \text{ T}$ with $H \parallel c$, and temperatures from 5–77 K, providing a detailed picture of pinning effects. Optimized results of flux pinning, magnetic current densities $J_{\text{cm}}(H, T)$, critical transition temperatures (T_c), lattice parameters, and microstructures are presented. The temperature dependence of the current density, $J_c(T)$, is mathematically modeled to compare the isotropic weak and anisotropic strong pinning contributions, for each of the mixed phase systems studied.

12:00 PM

(EMA-S15-017-2017) Correlation between Microstructure and Critical Current of heavily Zr-doped REBCO Superconductors over a broad range of temperature and magnetic field

E. Galstyan^{*†}; G. Majkic[†]; A. Xu[†]; M. Gharacheshmeh[†]; V. Selvamanickam[†]; I. University of Houston, USA

We report the microstructural and physical characteristics of high levels 15–25 mol % Zr-added $\text{REBa}_2\text{Cu}_3\text{O}_{7-x}$ (REBCO and RE = rare earth) coated conductors fabricated by Metal Organic Chemical Vapor Deposition (MOCVD). In this study, remarkable enhancements of the in-field critical current (I_c) and lift factor have been achieved in high magnetic fields up to 14 T between 77 K and 4.2 K. Moreover, we found a linear correlation between $I_c(77\text{K}, H \parallel c)$ and $I_c(T, H \parallel c)$ down to 4.2 K. The presence of strong flux pinning is attributed to the aligned 5–8 nm nanocolumns of BaZrO_3 and nanoprecipitates embedded in REBCO matrix with good crystal quality. The high Zr content was found to induce a high density of intrinsic defects, including stacking faults and dislocations. The correlation between improved in-field performance and microstructure will be discussed in this presentation.

12:15 PM

(EMA-S15-018-2017) Superconducting Joints between (RE) $\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ Coated Conductors via Solid State Bonding

C. Grimley^{*†}; J. Schwartz[†]; I. North Carolina State University, USA

One of the most promising commercially produced high temperature superconductors is (RE) $\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ (REBCO) in the form of a coated conductor (CC) on a Ni-alloy substrate due to high critical current and mechanical strength. Yet the inability to create low-cost superconducting joints remains a barrier in the use of REBCO CC for applications which require long conductor lengths. Current joining techniques use full or partial melting of the REBCO layer, which reduces the interfacial oxygen content, or a resistive solder. The resulting joints are either resistive or require a lengthy O_2 anneal to restore superconductivity. So far, no published work has attempted to directly bond REBCO CC's below the partial melt temperature of the material. Bonding in that region should maintain the oxygen content of the conductors, reducing the need for later annealing. The surface of the films contain localized variations in curvature which provide a driving force for solid state diffusion. These stresses can be enhanced by additional forces such as uniaxial pressure and an electric field. Here, we study the efficacy of this approach with and without field enhancements. We demonstrate the superconductivity of the joints and probe the relationship between the process and joint critical properties by characterizing them using low temperature four point probe measurements and electron microscopy.

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Advanced Electronic Materials: Multiferroic/Magnetic

Room: Indian

Session Chairs: Matthew Rosseinsky, University of Liverpool; Vladimir Shvartsman, University of Duisburg-Essen

2:00 PM

(EMA-S1-025-2017) Scanning Probe Microscopy Studies of the Magnetoelectric Effect in Composite Multiferroic Ceramics (Invited)

V. Shvartsman^{*†}; H. Trivedi[†]; D. C. Lupascu[†]; I. University of Duisburg-Essen, Germany

The magnetoelectric (ME) effect, i.e. control of magnetization or polarization by an electric or magnetic field, respectively, has attracted growing attention nowadays. The largest ME effect at room temperature has been reported for composite multiferroics that consist of piezoelectric and magnetostrictive phases. The most of experimental studies have dealt with the macroscopic ME response. Here we present study of the ME effect at the local scale, using scanning probe microscopy techniques. Multiferroic composites consisting of magnetic hexaferrite ($\text{BaFe}_{12}\text{O}_{19}$ or $\text{SrFe}_{12}\text{O}_{19}$) or ferrite (CoFe_2O_4 or NiFe_2O_4) phase and ferroelectric (BaTiO_3) phase were studied. Piezoresponse force microscopy revealed both the intrinsic change of the local piezoelectric coefficient and modulation of the polarization switching dynamics by a magnetic field. The local ME effect was maximal in the vicinity of the interfaces between piezoelectric and magnetostrictive phases, which agrees with the strain–stress mediated character of the ME coupling in such composites. For the converse ME effect we observed changes in the magnetic domains configuration under an electric field. The effect depends on microstructure. Analysis of the field-induced magnetic domain walls displacement revealed a hysteretic change of magnetization that can be rationalized by existence of localized defects concentration.

2:30 PM

(EMA-S1-026-2017) Symmetry, calculation and synthesis in the search for room temperature multiferroic magnetoelectric oxides (Invited)

M. Rosseinsky^{*†}; I. University of Liverpool, United Kingdom

This presentation addresses the challenge of combining electrical polarisation and magnetisation in a single phase material at room temperature in both bulk and thin film materials. The control of octahedral tilting and cation ordering in epitaxial thin film heterostructures of iron-based perovskites is shown to integrate these properties (1). By using the crystallographic shear in the Ruddlesden-Popper family to replace cation ordering, we can achieve polarisation, magnetisation and magnetoelectric behaviour in a bulk oxide at room temperature without the need for layer-by-layer growth (2). Ceramic oxide materials with bulk switchable magnetisation and electrical polarisation that are magnetoelectrically coupled at room temperature will be presented (3). (1) J. Alaria et al., Chemical Science 2014, 5, 1599 (2) M.J. Pitcher et al., Science 2015, 347, 420 (3) P. Mandal, Nature 2015, 525, 363

3:00 PM

(EMA-S1-027-2017) Control of magnetism in magnetoelectric heterostructured materials

M. Staruch⁺; S. Cheng¹; K. Bussmann¹; P. Finkel¹; 1. U.S. Naval Research Laboratory, USA

Magnetoelectric heterostructures are of interest for a wide range of device applications including random access memory, power harvesting or conversion, and sensors. At NRL, we have been investigating ways to maximize coupling between magnetostrictive and piezoelectric elements that is essential for optimal device performance. In particular, this is approached by utilizing a relaxor ferroelectric single crystal with high temperature and voltage stability as the piezoelectric phase. In this presentation, the impact of the piezomagnetic properties of the magnetostrictor will be examined as well as the potential of high coupling when driving the ferroelectric crystal through an induced phase transition, with converse magnetoelectric coupling coefficients of up to 3.5×10^{-6} s/m revealed.

3:15 PM

(EMA-S1-029-2017) Magnetic Ion Partitioning as a Mediator for Multiferroic Behaviour in Aurivillius Bismuth Iron Manganese Titanate

L. Keeney²; R. Whatmore¹; A. Faraz²; M. Schmidt²; C. Downing³; V. Nicolisi³; M. E. Pemble²; 1. Imperial College London, United Kingdom; 2. Tyndall National Institute, University College Cork, Ireland; 3. Trinity College Dublin, Ireland

Single-phase, RT ferroelectric (FE) / ferromagnetic (FM) multiferroics are needed for applications in data storage. We have made layered Aurivillius oxide films accommodating both FE and FM cations by chemical solution deposition (CSD) and liquid injection chemical vapour deposition (LICVD). We have demonstrated that films with an approx. composition $\text{Bi}_6\text{Ti}_3\text{Fe}_{1.5}\text{Mn}_{0.5}\text{O}_{18}$ (B6TFMO) with the 5- perovskite-layer structure are genuine, single-phase multiferroics in which magnetic fields can switch ferroelectric domains. Here, recent results are presented of atomic resolution cation analyses using a Nion ultra-STEM that show clear evidence for the partitioning of the magnetic cations (Mn and Fe) to the central three of the five perovskite layers, with a clear preference for the central layer. The potential reasons for this partitioning and its implications for multiferroicity will be discussed.

Reliability of Electronic Materials and Devices

Room: Indian

Session Chairs: Rajan Tandon, Sandia National Laboratories; Eugene Furman, Pennsylvania State University

3:45 PM

(EMA-S1-030-2017) Enhanced Electrical and Mechanical Properties of Coated Glass Ribbon (Invited)

M. Sarkarat¹; R. Rajagopalan¹; M. Yuan¹; E. Furman⁺; M. Lanagan¹; 1. Pennsylvania State University, USA

Alkali-free thin glass exhibits high dielectric breakdown strength (11-14 MV/cm), outstanding volumetric energy density (38 J/Cm³) and excellent high temperature performance. Hence, it is a potential candidate for high temperature power electronic capacitors. However, in order to improve reliability of manufactured wound glass capacitors, it is important to achieve mechanical stability along with self-clearing phenomenon in glass. In this presentation it will be shown that thin polymer coatings are capable of improving electrical and mechanical characteristics of glass capacitors. Polyurethane and fluorene-polyester coatings were deposited with dip coating. We The bending strength of polyurethane-coated glass was almost doubled while the bending radius was decreased by 2 times when 0.1 – 1 μm thick polymer was deposited on glass. The polymer coatings can heal existing defects on the surface and edge of the glass

thereby improving the mechanical properties. In the case of fluorene-polyester, a significant improvement of Weibull modulus over a wide temperature range was observed from a lesser contribution of extrinsic defects. For both types of coatings, the dielectric properties such as permittivity and loss of the glass were comparable to the pristine glass.

4:15 PM

(EMA-S1-031-2017) Lessons Learned from Failure Analyses of Electronic Components (Invited)

R. Tandon⁺; 1. Sandia National Laboratories, USA

Passive electronic components are multi-material assemblages, with many different ceramics and glasses. Accelerated aging and over-tests are employed prior to product acceptance. Failure analysis provides important insights into improving materials, processes or designs. Lessons learned from four failures are described. Optical and SEM fractography, strength testing, and fracture mechanics principles were employed to understand the causes. The first two examples are classical brittle failures: failure of a single crystal quartz resonator in mechanical shock was attributed to a defect missed during inspection, and failure of polycrystalline alumina in a thick-film resistor during vibration loading was attributed to excessive bending. The third case is a “glue-spalling” failure of a thick film resistor during thermal cycling. The final study describes the failure of a glass-body diode which is attributed partly to strain imposed due to the protective polymer coating during thermal cycling. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:45 PM

(EMA-S1-032-2017) Reliability of Analog Memory Storage using a Ferroelectric Capacitor

J. T. Evans⁺; 1. Radiant Technologies, Inc., USA

A functional memory storing analog states in a ferroelectric capacitor has been described in previous EMA meetings. An autonomous memory circuit consisting of a conductive load, the ferroelectric capacitor, and a current controlled switch such as a bipolar transistor or a current mirror FET pair will implement analog storage and recall in a ferroelectric capacitor. Given the long struggle to limit the negative effect of imprint on the reliability of destructive-read binary-storage ferroelectric random access memories (FRAMs), how will imprint affect the reliability of analog data stored in a ferroelectric capacitor? Can the analog state of a ferroelectric capacitor be successfully discriminated at 70°C or 85°C for ten years? The answer depends upon the number of analog states into which the remanent polarization of the capacitor is divided. Radiant Technologies has successfully tested analog memory reliability over temperature of 3-states stored in PZT capacitors. The author will analyze those results.

5:00 PM

(EMA-S1-033-2017) Resistance Degradation and Polarization Effects on the Fermi level at the Barium Titanate/ Nickel Interface

D. Long⁺; A. Klein²; E. C. Dickey¹; 1. North Carolina State University, USA; 2. Technical University Darmstadt, Germany

Barium titanate (BTO) dielectric layers and nickel electrodes are integral components in multilayer ceramic capacitors (MLCCs). MLCC performance is determined by the magnitude and stability of its capacitance and leakage current; the latter of which is largely controlled by the schottky barrier at the metal/dielectric interface. Here we study the position of the Fermi level, E_F , of the BTO/Nickel interface as a function of ferroelectric polarization and resistance degradation. X-ray Photoelectron Spectroscopy was employed to study E_F and chemistry of the interface. 4 nm nickel electrodes were

sputtered in an ultrahigh vacuum system on 5 x 5 x 0.5 mm undoped (100) oriented single crystal BTO substrates. The initial poling treatment caused a permanent shift in E_F which increased the schottky barrier. This initial shift can arise from interfacial defect states or from domains changing from a multidomain state to a more ordered state with polarizations aligning with the electric field. Switching the ferroelectric polarization after the first poling had a negligible effect on E_F . Electrical degradation performed at 40 V (800 V/cm) at 210°C enhanced the leakage current over time, and led to a diminished schottky barrier. Samples with 25 nm nickel electrodes were also studied for their ferroelectric and degradation properties and no effect of electrode thickness was found.

5:15 PM

(EMA-S1-034-2017) Evaluation of Fabrication Induced Damage on the Ferroelectric & Piezoelectric Lead Zirconate Titanate (PZT) Thin Films for Clamped and Unclamped Final Devices

M. Rivas^{*1}; R. Q. Rudy²; B. D. Huey¹; R. G. Polcawich²; 1. University of Connecticut, USA; 2. U.S. Army Research Laboratory, USA

Ferroelectric and piezoelectric thin films are vital components for a number applications such as ferroelectric memory, RF devices, and various other microelectromechanical systems (MEMS). The ferroelectric and piezoelectric performance of thin film $\text{Pb}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$ (PZT) MEMS can be affected by the device design as well as by the presence of substrate clamping effects. To understand these effects, the dielectric and ferroelectric properties of PZT thin films are tracked throughout a MEMS fabrication process for circular capacitor structures and rectangular structures that will become fully released (unclamped) cantilever structures. The clamped capacitors and the unclamped cantilevers are co-located and separated by 100 μm . The structures consist of a 500nm thick elastic layer of SiO_2 , a bottom electrode of (111) textured Pt, an approximately 500nm thick PZT (52/48) thin films deposited via chemical solution deposition, and either Pt or IrO_2 top electrodes with a thickness of 100nm. Project data shows different hysteresis behavior, up to 27% change in maximum polarization, a 7% change in maximum permittivity, and 11% dielectric loss difference between the clamped and unclamped structures. Differences in behavior throughout the fabrication process for devices with IrO_2 or Pt top electrodes will also be described.

5:30 PM

(EMA-S1-035-2017) Impact of charge injection into bulk dielectric capacitors on the resistance degradation process

T. J. Bayer^{*1}; J. Wang¹; J. Carter¹; R. Wang¹; L. Chen¹; C. Randall¹; 1. Pennsylvania State University, USA

Charge injection is a highly undesirable process in capacitor applications as it increases the leakage current. For bulk single crystal capacitors the impact is usually believed to be negligible. Hence the established resistance degradation model includes the assumption that the condition of local defect equilibrium is established immediately after the oxygen vacancy migration throughout the entire degradation process. In-situ impedance studies of Fe-doped SrTiO_3 single crystals and corresponding simulations demonstrated that the condition of local defect equilibrium is only fulfilled for sufficiently advanced degradation states. Experimentally observed impedance features at the beginning of the degradation do not match the resistance degradation model. Here, we present simulated impedance features based on the assumption of an increased charge injection at the cathode interface with degradation time. We will show that simulations based on charge injection provide a very good match with experiments. The results demonstrate that the initial resistance degradation process is influenced by both charge injection and oxygen vacancy migration. This finding is very important as the charge injection process changes the local electric field distribution and thus impacts the oxygen vacancy migration. Resulting consequences will be presented.

S2: Advanced Processing for Electronic and Electrochemical Systems: Crystals, Films and Devices

Interface Engineering and Characterization for Novel Properties or Improved Stability

Room: Coral B

Session Chair: Mark Losego, Georgia Institute of Technology

2:00 PM

(EMA-S2-028-2017) Alumina-Silicon Interfaces: Understanding the Origins of Fixed Charge and the Influence of Non-Hydrolytic Deposition Chemistries (Invited)

N. C. Strandwitz^{*1}; 1. Lehigh University, USA

Interfaces between semiconductors and oxides are important for an array of applications including surface passivation layers on solar cells and gate dielectrics. Fixed negative charges are often found at alumina-silicon interfaces as evidenced by ex situ analyses. We utilize the temporally-separated chemical events that result in ALD growth to study the evolution of fixed charge in situ during deposition. Here, the conductance across a Si channel region was measured during ALD of aluminum oxide and yielded information about the effects of ALD chemistry on the charge carrier concentrations in the channel. We observed evidence for the formation of a small fixed negative charge upon the first chemisorption of trimethylaluminum on the Si/ SiO_2 surface. There is also significant interest in minimizing oxidative damage to substrate semiconductors during ALD. Non-hydrolytic (NH) ALD chemistries utilize oxygen sources other than water or oxygen and have been shown inflict less oxidative damage to substrates. We directly compare NH and traditional ALD chemistries and have found the NH ALD films have a larger fixed negative charge and larger interface trap state density. The understanding and control of semiconductor-dielectric interfaces is critical for controlling the flat band voltage in gating applications and for passivation in photovoltaics.

2:30 PM

(EMA-S2-029-2017) Investigation of native defects states in the HfO_2 by DLTS

A. Kumar^{*1}; S. Mondal¹; K. Koteswara Rao¹; 1. Indian Institute of Science, India

HfO_2 have appeared as the key gate dielectric to substitute the traditional SiO_2 . A large number of theoretical works is present in the literature dealing with the detailed analysis of oxygen vacancy related trap in HfO_2 , while experimental estimations are few. In this work, the defects present in the HfO_2 gate dielectric and at the Si/ HfO_2 interface is experimentally probed by DLTS technique. The traps present in the bulk HfO_2 or in the close vicinity of the interface communicate with the interfacial traps (as they are in the range of tunneling/hopping distances), finally with the conduction or valence bands of Si. We observe four prominent defect states and believe all these are related to oxygen vacancy in different charge states. The activation energies of trap states are in the range of 1.2 – 2 eV from the HfO_2 conduction band edge and they fall within the forbidden region of the band gap of Si in the band alignment of Al/ HfO_2 /Si gate stack. The capture cross-sections of these states fall in the range of ($\sim 10^{-18}$ - 10^{-19} cm^2), which indicate a minor impact on the device operation.

2:45 PM

(EMA-S2-030-2017) Advantages of PEALD Dielectrics on GaN Materials (Invited)

B. S. Eller¹; M. Hao¹; S. Chowdhury²; R. Nemanich^{*1}; 1. Arizona State University, USA; 2. University of California - Davis, USA

The performance of GaN devices is degraded by a high concentration of defects at the dielectric/GaN interface, which results in reliability issues, i.e. gate leakage and current collapse. The defects responsible for these failure mechanisms are likely related to the surface and interface charge that compensate the strong spontaneous polarization of GaN ($\sim 1.81 \times 10^{13}$ charges/cm²); but research indicates these failure mechanisms can be at least partially mitigated with appropriate cleaning processes and gate dielectric. Plasma-enhanced ALD (PEALD) for dielectric deposition uses oxygen plasma as the oxidant, which offers significant advantages over other ALD techniques as well as non-ALD techniques, including lower impurity content, improved stoichiometry, lower deposition temperature, and versatility. Some of the most promising PEALD dielectrics include Al₂O₃ and SiO₂. Our research has worked to investigate ALD-Al₂O₃-SiO₂/GaN interfaces with particular attention to the influence of surface preparation, gate dielectric and dielectric passivation growth conditions, as well as post deposition annealing on interface states. In our specific work, in-situ photoelectron spectroscopy in conjunction with ex-situ electrical characterization has been used to examine the relevant interface for high-powered applications. This research is supported by the ONR DEFINE MURI and ARPA-E Switches Programs.

Interface Engineering for Novel Properties or Improved Stability

Room: Coral B

Session Chair: Christina Rost, University of Virginia

3:45 PM

(EMA-S2-031-2017) Tuning the Surface of Fe-doped NiO Nanoparticles for Oxygen Evolution Reaction Electrocatalysis (Invited)

E. Lucas¹; B. Lynch¹; J. Tracy¹; V. Augustyn^{*1}; 1. North Carolina State University, USA

The efficient electrocatalysis of the oxygen evolution and reduction reactions (respectively, OER and ORR) remains a serious challenge for the development of electrochemical energy conversion and storage devices such as fuel cells, electrolyzers, and metal-air batteries. New non-noble metal catalysts and improved understanding of their interfacial mechanisms are necessary. Fe-doped nickel oxides and hydroxides are the most active non-noble metal electrocatalysts for the OER in alkaline electrolytes. Nanostructured forms of these materials offer high surface areas, which are necessary for high areal current densities. However, it is not clear how the surface chemistry and surface defects of these nanostructures, including the presence of organic ligands or dopants, influence the electrochemical reaction occurring on the nanomaterial/electrolyte interface. This presentation will describe how the surface of Fe-doped NiO nanoparticles can be tuned to yield stable and reproducible electrocatalytic activity at low overpotentials. The electrochemical response is correlated with the surface chemical composition and local structure using, respectively, X-ray photoelectron spectroscopy and Raman microscopy. The results underscore the high sensitivity of electrocatalysis to the surface chemistry and defects of nanomaterials.

4:15 PM

(EMA-S2-032-2017) Tuning the Electronic Ground State of Ca₂RuO₄ using Epitaxial Strain (Invited)

H. Nair^{*1}; J. Ru²; Y. Liu³; N. Shukla⁴; B. Grisafe⁴; C. S. Chang²; Q. Han⁶; A. Millis⁵; D. A. Muller²; S. Datta⁴; K. Shen²; D. G. Schlom¹; 1. Cornell University, USA; 2. Cornell University, USA; 3. Zhejiang University, China; 4. University of Notre Dame, USA; 5. Cornell University, USA; 6. Columbia University, USA

Sizable strain tuning of a metal-insulator transition (MIT) has been a holy grail of condensed matter physics for decades. Bulk single crystal Ca₂RuO₄ undergoes an MIT at 357 K and becomes an antiferromagnet with a Neel temperature of 110 K. By leveraging tensile strain in our molecular beam epitaxy grown Ca₂RuO₄ thin films, we have pushed this MIT to above 600 K compared to 357 K for bulk single crystals. Moreover, the MIT can be electrically triggered making Ca₂RuO₄ a very attractive candidate for Mott-based electronics, which require devices to operate above 400 K. On the compressive strain side we have been able to suppress MIT to ~ 200 K. Preliminary calculations confirm our experimental findings that the electronic ground state in Ca₂RuO₄ is extremely sensitive to strain. Until now, such a dramatic effect of strain on the ground state electronic properties has not been observed in any other material system making Ca₂RuO₄ an excellent candidate for further explorations of strain-induced tuning of electronic properties.

4:45 PM

(EMA-S2-033-2017) Mechanisms of defect suppression at the initial stages of La₂MnNiO₆ film growth

P. Sushko^{*1}; S. Spurgeon¹; Y. Du¹; T. Droubay¹; A. Devaraj¹; P. Longo³; S. Chambers²; 1. Pacific Northwest National Lab, USA; 2. Pacific Northwest National Laboratory, USA; 3. Gatan Inc., USA

La₂MnNiO₆ (LMNO) is a ferromagnetic semiconductor with a theoretical magnetic moment of 5 μ_B per formula unit; however, molecular beam epitaxy (MBE) grown films exhibit a much lower magnetic moment, which has been attributed to extended defects [1]. Here we focus on the initial stages of LMNO growth and atomic-scale mechanisms of defect formation near the film/substrate interface. We find that LMNO grown on SrTiO₃ (STO) has no detectable defects in the 3-5 nm region near the interface, while NiO inclusions begin to appear at larger distances. Ab initio simulations of prototype point defects as a function of LMNO thickness suggest that at MBE-grown LMNO films contain oxygen vacancies, which, in turn, promote the formation of Mn-Ni anti-site defects. At the same time, the STO substrate acts as an additional oxygen reservoir; oxygen diffusion from the substrate to the near-interface region of the film annihilates the vacancies and restores the ideal Mn-Ni ordering. As the film thickness increases, this process is suppressed, thus creating conditions in which isolated vacancies and anti-site defects can accumulate and transform into large-scale lattice defects. These results suggest that substrates that can readily donate oxygen to the films could lead to high-quality films, albeit at the expense of the quality of the substrate, and vice versa. [1] S R Spurgeon, et. al., Chem. Mater. 28, 3814 (2016).

5:00 PM

(EMA-S2-034-2017) Imaging and Quantifying Changes at Magnetic and Magnetoelectric Interfaces (Invited)

M. B. Holcomb^{*1}; 1. West Virginia University, USA

The interfaces between magnetic and ferroelectric materials may hold the key to strong electrical control of magnetism. We explore such a system (La_{0.7}Sr_{0.3}MnO₃/PbZr_{0.2}Ti_{0.8}O₃ thin films) through synchrotron imaging and our newly developed technique resulting in depth-dependent absorption spectroscopy. Imaging of the individual layers and the resulting interface allows quantitative determination of uncompensated Ti spins and their relative local orientation with respect to the ferromagnetic direction. A preference for perpendicular coupling is observed, as seen in the biquadratic coupling in

some metallic systems. Our depth dependent spectroscopy results are obtained by comparing theoretical models to experimental data obtained utilizing two techniques (total electron yield and fluorescence) with different probing depths. As it is strongly correlated with the magnetic behavior, I will discuss the effect of several parameters on the depth-dependent Mn valence in the $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ thin films. While the imaging and depth-dependent measurements will be described for this research, these techniques could be widely used in various other materials and potentially other science research. We are also applying similar depth-dependent approaches to magnetic thin films to understand how their properties vary with depth.

5:30 PM

(EMA-S2-035-2017) Assembly of Magnetoelectric Nanowires into Magnetic Field Sensors

M. J. Bauer^{*1}; X. Wen²; P. Tiwari¹; D. P. Arnold²; J. S. Andrew¹; 1. University of Florida, USA; 2. University of Florida, USA

Magnetoelectric materials are functional materials in which a magnetic field can control an electrical polarization and conversely an applied voltage can control magnetization. It has been predicted that freestanding magnetoelectric composites could achieve magnetoelectric coefficients orders of magnitude greater than thin films due to a reduction in substrate clamping. Here, we have synthesized freestanding magnetoelectric nanofibers consisting of a cobalt ferrite magnetostrictive phase and a barium titanate piezoelectric phase with the potential to exhibit magnetoelectric coefficients orders of magnitude greater than thin films. These nanofibers have been assembled onto metal electrodes on silicon using dielectrophoresis. The effects of synthesis conditions on nanowire morphology and magnetoelectric properties will be presented along with the key parameters for dielectrophoretic nanofiber assembly. Lastly, the dielectric, magnetic and magnetoelectric properties of the nanofiber and nanofiber-based devices will be presented.

S4: Computational Design of Electronic Materials

Materials by Design II

Room: Coral A

Session Chair: Rohan Mishra, Washington University, St. Louis

2:00 PM

(EMA-S4-008-2017) Closing the loop between materials modeling and neutron scattering data (Invited)

T. Proffen^{*1}; 1. Oak Ridge National Lab, USA

Neutron scattering enables simultaneous measurement of structural and dynamic properties of materials from the atomic scale (0.1 nm, 0.1ps) to the meso scale (1μm, 1us). These ranges are remarkable complementary to current capabilities of computational modeling and the simplicity of the scattering cross section allows the prediction of neutron scattering data straight forwardly from computer modeling results. Oak Ridge National Laboratory is home to two world leading neutron facilities, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) as well as the Oak Ridge Leadership Computing Facility. Turning these ORNL's unique strengths into the highest impact science is not without challenges. In this talk I will discuss challenges and opportunities and present recent advances at the SNS towards linking materials simulation and neutron scattering and towards real time feedback between experiment and simulation.

2:30 PM

(EMA-S4-009-2017) Learning from data to design materials (Invited)

T. Lookman^{*1}; 1. Los Alamos National Laboratory, USA

A key aspect of accelerating the materials discovery process is learning from data to guide the next experiments towards materials with desired properties. Needed are tools that will seamlessly integrate data with theory and inference in a codesign loop for prediction and understanding. I will discuss a couple of examples, including piezoelectrics and alloys, where we lay out an approach to address this challenging question.

3:00 PM

(EMA-S4-010-2017) Exploring CdZnTeSe alloys for improved room temperature radiation detectors through first-principles calculations (Invited)

J. B. Varley^{*1}; 1. Lawrence Livermore National Laboratory, USA

Cadmium Zinc Telluride (CZT) alloys are currently the state-of-the-art choice for room-temperature radiation detectors owing to favorable properties such as an increased band gap and a large carrier mobility (μ) and carrier lifetime (τ) that facilitate efficient charge collection. Despite their appeal, the difficulty in growing large, uniform CZT crystals has led to high material costs that have limited the widespread adoption of CZT detectors. Alloys incorporating Se have also garnered interest due to experimental demonstrations of high $\mu\tau$ (up to $10^{-2} \text{ cm}^2/\text{V}$) in $\text{CdTe}_{1-y}\text{Se}_y$ (CTS) alloys, but suffer from a reduced band gap. Adding some Zn may therefore be desirable to increase the band gap while hopefully maintaining the excellent charge transport. Here we use hybrid functional calculations to computationally assess the properties of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}_{1-y}\text{Se}_y$ alloys as a function of composition to improve the development of alloys with favorable electronic properties. Our calculations characterize the electronic structure and thermodynamic stability of solid solution alloys over the entire quaternary space and identify compositions that exhibit favorable properties for alternatives to pure CZT or CTS. This work was performed in collaboration with V. Lordi, U.N. Roy and R.B. James, prepared by LLNL under Contract DE-AC52-07NA27344 and funded by the U.S. DOE/NNSA DNN R&D.

4:00 PM

(EMA-S4-011-2017) Bismuth halide semiconductors as nontoxic alternatives to lead halide perovskite photovoltaics (Invited)

R. Mishra^{*1}; X. Huang¹; A. S. Thind¹; Y. Myung¹; S. Huang²; G. Pilania³; P. Banerjee¹; 1. Washington University in St. Louis, USA; 2. Washington University in St. Louis, USA; 3. Los Alamos National Lab, USA

The power conversion efficiency of lead halide perovskite solar cells is now close to 25%. However, they are plagued with environmental and thermodynamic instability, which combined with the highly toxic nature of lead, makes them less attractive for commercialization. Bismuth is one atomic number higher than lead and is significantly less toxic. In this talk, examples of various bismuth halides that can serve as lead-free alternative photovoltaic materials will be discussed. Specifically, combined experimental and theoretical results demonstrating the defect-tolerant behavior of bismuth iodide nanoplates that enables remarkably fast and sensitive photoresponse behavior will be shown. Theory-guided tuning of band gap in stable ternary bismuth halides with layered structures will be discussed. Finally new and stable quaternary bismuth-based compounds optimized for photovoltaic applications predicted using data-mining and density functional theory calculations will be presented, highlighting the potential of bismuth halide photovoltaics.

4:30 PM

(EMA-S4-012-2017) Exotic Elastic Properties of Layered Two-dimensional Materials (Invited)

S. Woo^{*1}; 1. Korea Institute for Advanced Study, Republic of Korea

We have investigated the elastic properties of two-dimensional layered materials including graphene, h-BN and 2H-MoS₂ using First-Principles calculations. Layered materials, due to their strong anisotropy and interlayer van der Waals interaction, show exotic mechanical properties compared to typical bulk crystals. First interesting thing is that a multilayered graphene is directionally auxetic; its Poisson's ratio along the out-of-plane direction is negative while h-BN and 2H-MoS₂ show near zero and positive Poisson's ratio respectively, spanning all possibilities of sign of the ratios. While the in-plane Poisson's ratios are all positive regardless of their disparate electronic and structural properties, the characteristic interlayer interactions as well as layer stacking structures are shown to determine the sign of their out-of-plane ratios. Such exotic elastic property can be understood by looking at the electronic orbital properties carefully. Second, I will also present an interesting shear elastic properties of the layered materials. The strain-induced polarization, piezoelectricity, causes coupling between shear and tensile strains in the context of Berry's phase. Recently an unexpected trend of interlayer shear mode frequency splitting was observed in a Raman experiment of MoS₂ under tensile strain. Our theory bridges the experiment with strain induced interlayer shear sliding.

5:00 PM

(EMA-S4-013-2017) Modeling multicomponent circuits in ZnO/graphene nanocomposites: A bottom-up approach

I. C. Cezário^{*1}; D. Muller²; F. R. Moreira²; G. A. de Barros²; H. P. Roldán²; C. R. Rambo²; 1. Federal University of Santa Catarina, Brazil; 2. Federal University of Santa Catarina, Brazil; 3. Federal University of Santa Catarina, Brazil

Nanocircuits are being developed for diverse applications from increasing computer performance to new tools for medicine and especially in nanoelectronics. In this work, bulk ZnO/Graphene nanocomposites were produced through an in situ sol-gel method, followed by controlled drying. The nanostructured gels were electrically characterized through I-V curves under different input conditions and their behavior was modelled using multicomponent circuits where the synthesis parameters, final compositions and working electrodes could be related to the elements of the equivalent integrated circuit. Graphene (50-100 nm) with concentrations in the range of 1-10 wt.% was in situ incorporated into zinc oxide gel precursor during gel synthesis. The nanocomposites were characterized according to the crystalline structure and surface area. Modeling of the electrical behavior of the composite was performed using PSpice software. Results revealed that discrete electronic models could be extracted from the nanocomposites.

5:15 PM

(EMA-S4-014-2017) A first-principles understanding of the structure-property relationships in polymorphic MoO₃

J. Yun^{*1}; W. Jang¹; T. Lee¹; Y. Lee¹; A. Soon¹; 1. Yonsei University, Republic of Korea

Molybdenum trioxides (MoO₃) have been suggested as potential materials for key opto-electronic applications due to their proper band edge positions and appropriate band gap sizes. However, the relationship between these polymorphic phases and their electronic structures is not well known. Namely, the influence of the delicate interplay of MoO₆ octahedron tilting and the metal cation off-center displacement is poorly understood. In this work, by using first-principles density-functional theory calculations, we investigate the thermodynamic stability of various polymorphic MoO₃ and study their electronic band structure. Specifically, we systematically analyze the internal (i.e. non-centrosymmetry of cation) and external (i.e. octahedral tilting) distortions via the quadratic elongation and

bond angle variance methods. Here, we report how the structural factors in these polymorphic MoO₃ can substantially dictate their electronic structure and thus provide a structure-property design map for advanced functional oxides in opto-electronic applications.

5:30 PM

(EMA-S4-015-2017) Modelling New Absorbers Materials for More Efficient Solar Energy Use

P. Wahnou^{*1}; P. Palacios¹; J. Conesa²; E. Menendez-Proupin²; 1. Universidad Politécnica de Madrid, Spain; 2. Universidad de Chile, Chile; 3. Instituto de Catalisis y Petroleoquímica-CSIC, Spain

We present several materials actively studied by our groups as good absorbers for photovoltaic applications. These materials, have been proposed to boost photovoltaic efficiency through coupling the absorption of two low energy photons to achieve a higher energy electron excitation. We have verified with accurate DFT calculations and beyond, that semiconductors as chalcopyrite CuGaS₂, spinel In₂S₃ or layered SnS₂ can provide this situation when a cation in their structure is partially substituted by an element such as transition metal (TM). Band alignments of the heterojunctions between new proposed absorbers and different semiconductors have been obtained using an average electrostatic potential as reference level. Other material actively studied is the perovskite (CH₃NH₃PbI₃). We have computed its electronic structure and relevant properties of the orthorhombic phase using hybrid functional combining spin-orbit effects. The computed binding energy of the unrelaxed exciton agrees with recently reported experimental data. Fast dynamics and large diffusion lengths of the current carriers are key for the high photovoltaic efficiencies shown by these materials. Experimental work made via wet chemistry methods has been done for several of these materials. These studies verify that new absorption features appear in the optical absorption spectrum which matches the predicted DFT-based theoretical absorption results.

5:45 PM

(EMA-S4-016-2017) Study of a SnSbCu soldering alloy for electronic components assembly

M. Wary^{*1}; R. Pesci¹; 1. Arts et Métiers ParisTech, France

Lead and lead containing materials are considered to be a major threat to human health and the environment. EU directive RoHS prohibited the use of lead-containing solders, especially in the electronics industry. In the studied context, it is essentially the soldering alloys for the assembly of components on electronic boards that fall under this directive because they contain lead. If some reliable solutions were founded for low temperatures applications to replace PbSn eutectic alloy, there is a lack for higher temperatures applications since the properties of possible substitutes are not well known. It is on the findings of an European project, COST MP HISOLD 0602, that we relied to offer a SnSbCu type alloy as a possible alternative. Its behaviour is not well known; the aim here is to study the properties of this alloy for potential future use as a substitute. First by modelling its exact chemical composition in relation to the expected properties, and then by characterising it completely through comprehensive experimental approaches: melting point (DSC), conductivities, characterisation of the final chemical composition, microstructure and its evolution during thermal aging (SEM+EDS, X-ray fluorescence) as well as mechanical properties (microhardness, tensile and creep tests).

S6: Fundamentals to Applications for the Use of Thermal Energy for Power Generation and Refrigeration

Use of Thermal Energy

Room: Mediterranean C

Session Chair: Brian Donovan, United States Naval Academy

2:00 PM

(EMA-S6-001-2017) Perspectives for High Temperature Thermoelectric Applications and Development of Materials (Borides, Sulfides, Oxides, and Nitrides) (Invited)

T. Mori^{*1}; 1. National Institute for Materials Science (NIMS), Japan

Thermoelectric materials are being actively developed now, utilizing state-of-the-art nanotechnology, novel concepts and novel materials [1]. It may not be widely known, due to the straightforwardly relatively high efficiency of turbines, but one especial need exists to develop TE materials which can utilize high temperature unutilized/waste heat in thermal power plants, steelworks, factories, incinerators, etc. and also focused solar power [2]. The thermal power plant application will especially need ultra-high temperature TE materials. We have been particularly interested in developing the properties of inorganic and refractory materials mainly composed of abundant, inexpensive elements (so-called "Element Strategy") like borides, silicides, sulfides, oxides, nitrides, by utilizing and controlling particular features of the crystal structure and structure-property relationships [3]. I will give an overview of this strategy, together with the recent developments we have made in further developing various promising boride [4], sulfide [5], oxide [6], and nitride [7] compounds for thermoelectrics.

2:30 PM

(EMA-S6-002-2017) Zintl thermoelectrics: Transport engineering through crystal chemistry (Invited)

A. Zevalkink^{*1}; 1. Michigan State University, USA

Intermetallic Zintl phases form complex composite structures characterized by covalently-bonded polyanions stabilized by the surrounding cations. Zintl polyanions occur in an astounding variety of forms, including isolated 0-dimensional clusters, 1-D chains, and 2-D slabs, which leads to extremely anisotropic structures in some instances. Excellent high temperature thermoelectric performance and stability in many Zintl compounds has inspired a recent surge of interest in Zintl phase thermoelectrics. Understanding the influence of the complex crystal chemistry in Zintl phases on their thermal and electronic transport properties is critical to engineering materials with improved thermoelectric efficiency. Our exploration of structurally complex ternary Zintl antimonides as novel thermoelectric materials has demonstrated that such phases meet many of the fundamental requirements for high thermoelectric efficiency: glass-like lattice thermal conductivity, a band gap in the electronic structure, and tunable electronic properties. By exploiting defect structures or by using traditional doping and alloying approaches to adjust and optimize the Fermi level, a diverse class of promising new thermoelectric materials has been developed and optimized.

3:00 PM

(EMA-S6-003-2017) Thermoelectric properties of GdCuTe₂ compounds

J. S. Vaney^{*1}; E. Benson¹; T. Mori¹; 1. National Institute for Materials Science (NIMS), Japan

Compounds of composition ABX₂ (with A,B as rare earths or transition metals and X as chalcogenides) have recently been attracting attention as thermoelectric materials [1,2]. A number of these compounds display very low thermal conductivities (< 0.5 W.m⁻¹.K⁻¹) and promising ZT values have been reported for some of them,

such as TmAgTe₂ or YCuTe₂ [3,4]. GdCuTe₂ is a monoclinic layered compound that crystallizes in the C2/m space group. As for some other compounds of ABX₂ type, this composition shows a very low thermal conductivity (0.5 W.m⁻¹.K⁻¹ at 300 K), which, together with a Seebeck coefficient of ~200 μV.K⁻¹, allows to reach a moderate ZT value near 0.1 at 300 K. We also present here the beneficial effect of the substitution of Dy for Gd in the system Gd_{1-x}Dy_xCuTe₂ on the thermoelectric properties of the compound, as well as the dependence of the properties on Gd atom filling on the crystallographic 2i site in this system.

3:15 PM

(EMA-S6-004-2017) Influence of chemical ordering on the thermal conductivity and electronic relaxation in FePt thin films in heat assisted magnetic recording applications

P. Hopkins^{*1}; A. Giri²; 1. University of Virginia, USA; 2. University of Virginia, USA

We report on the out-of-plane thermal conductivities of tetragonal L10 FePt (001) easy-axis and cubic A1 FePt thin films via time-domain thermoreflectance over a temperature range from 133K to 500K. The out-of-plane thermal conductivity of the chemically ordered L10 phase with alternating Fe and Pt layers is ~23% greater than the thermal conductivity of the disordered A1 phase at room temperature and below. However, as temperature is increased above room temperature, the thermal conductivities of the two phases begin to converge. Molecular dynamics simulations on model FePt structures support our experimental findings and help shed more light into the relative vibrational thermal transport properties of the L10 and A1 phases. Furthermore, unlike the varying temperature trends in the thermal conductivities of the two phases, the electronic scattering rates in the out-of-plane direction of the two phases are similar for the temperature range studied in this work.

Fundamentals of Thermal Energy

Room: Mediterranean C

Session Chair: Edward Gorzkowski, Naval Research Lab

4:00 PM

(EMA-S6-005-2017) Thickness and connectivity effects on the thermal conductivity of amorphous silicon: Insight into the fundamental nature and behavior of non-phonon vibrations in disordered structures (propagons, diffusons and locons)

J. Braun¹; A. Giri¹; J. Gaskins¹; H. Fujiwara²; P. Hopkins^{*1}; Z. Leseman³; P. E. Norris¹; 1. University of Virginia, USA; 2. Gifu University, Japan; 3. Kansas State University, USA

Phonons only exist in periodic systems. In disordered systems, such as glasses, the concept of a phonon is lost, and a new taxonomy for vibrational energy transport must be realized. While the thermal conductivity of glasses have been well modeled in the context of this classification, experimental realization of these vibrations along with observation of how these vibrations impact the thermal conductivity of amorphous solids have not been reported. Here, we reports on a series of experiments on amorphous silicon films in which we demonstrate evidence of these non-phonon modes. First, we investigate thickness-limited size effects on the thermal conductivity of amorphous silicon thin films, which is ascribed to boundary scattering of long wavelength vibrations and an interplay between the energy transfer associated with propagons and diffusons. Next, we demonstrate a novel way to reduce thermal conductivity of fully dense (above the rigidity percolation threshold) amorphous thin films below the minimum limit by systematically changing the coordination number through hydrogenation. This further reduction in thermal conductivity beyond the fully dense limit is in direct correlation to changes in diffuson and locon interactions.

4:15 PM

(EMA-S6-006-2017) Probing anisotropic thermal conductivity of dielectric materials

B. Donovan^{*2}; A. Giri³; J. Gaskins³; E. Gorzkowski¹; P. Hopkins³; 1. Naval Research Lab, USA; 2. United States Naval Academy, USA; 3. University of Virginia, USA

In this study we utilize advance the highly sensitive thermal characterization technique, time domain thermoreflectance (TDTR), in order to gain sensitivity to anisotropic in-plane thermal conductivity of dielectric materials. With specific alterations to the optics used in typical TDTR, we gain sensitivity to in-plane thermal conductivity with distinct resolution in both of the principal in-plane directions of a single crystal specimen. We verify our measurements with single crystalline TiO₂ and demonstrate the ability to extend these measurements into relevant material systems such as thin film oxides and uniaxially and biaxially strained dielectric polymers.

4:30 PM

(EMA-S6-007-2017) Structure, bonding, and anharmonicity in tetrahedrite-based thermoelectrics (Invited)

D. Morelli^{*1}; 1. Michigan State University, USA

In order to function efficiently, thermoelectric materials require a unique combination of thermal and electronic transport properties. One important design criterion, for example, is to minimize thermal conductivity, and one very successful approach to achieving this condition is the concept of phonon-glass-electron-crystal (PGEC), in which localized phonon modes of guest atoms in cage-like structures, such as skutterudites and clathrates, induce strong phonon scattering. Using the family of tetrahedrite-based semiconductors as an example, we show that PGEC-like behavior can manifest itself in crystal structures that possess no noticeable cage-like structure. Using a combination of theoretical calculations, x-ray and neutron probes, and thermal and electronic characterization, we show that this PGEC-like behavior in tetrahedrites has its origin in a unique set of structural and bonding aspects that give rise to strong lattice anharmonicity and low lattice thermal conductivity. This low thermal conductivity, in concert with a favorable band structure, endows tetrahedrite with a thermoelectric figure of merit rivaling that of PbTe. Because tetrahedrite contains no toxic or rare elements, it is a strong competitor as a low cost, environmentally benign material for thermoelectric power generators.

5:00 PM

(EMA-S6-008-2017) Positive Thermal Conductivity Change in PZT Thin Films Under Applied Fields via Substrate Clamping Relief

J. Ihlefeld^{*1}; B. Foley²; M. Wallace³; D. Medlin¹; D. Scrymgeour¹; B. McKenzie¹; J. Michael¹; E. A. Paisley¹; S. Troler-McKinstry³; J. Gaskins²; P. Hopkins²; 1. Sandia National Laboratories, USA; 2. University of Virginia, USA; 3. Pennsylvania State University, USA

Manipulating thermal conductivity in the solid state at room temperature is possible by utilizing reconfigurable domain boundaries in ferroelectrics. Initial results in this field utilized PZT bilayers where the thermal conductivity decreased under applied field owing to an increase in the numbers of ferroelastic domain boundaries. This increase in domain boundaries is believed to be related to substrate clamping. In this presentation we will show how removal of the underlying silicon substrate via microfabrication enables growth of domains, reduction in the numbers of domain walls, and an increase in thermal conductivity when under an applied field. We observe rapid and repeatable 13% changes in thermal conductivity in a 600 nm thick PbZr_{0.3}Ti_{0.7}O₃ thin film that was prepared into a membrane structure. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

5:15 PM

(EMA-S6-009-2017) Thermal Conductivity of Lead Zirconate Titanate (PbZr_{1-x}Ti_xO₃) Thin Films Across the Compositional Phase Diagram

B. Foley^{*3}; E. A. Paisley²; C. DiAntonio²; T. Chavez²; G. L. Brennecke¹; J. Gaskins³; J. Ihlefeld²; P. Hopkins³; 1. Colorado School of Mines, USA; 2. Sandia National Laboratories, USA; 3. University of Virginia, USA

A thorough investigation of the thermal conductivity (κ) of thin film lead zirconate titanate (PbZr_{1-x}Ti_xO₃, PZT) across the compositional phase diagram is presented. The films were deposited on platinumized silicon substrates via chemical solution deposition (CSD) and the thermal properties were measured using time domain thermoreflectance (TDTR). The asymmetry in κ as a function of x demonstrated in the PZT system is surprising compared to other alloy/solid-solution systems such as Si_xGe_{1-x} and Al_xGa_{1-x}N. This observation is explored in the context of the distinctly different trends for κ over temperature between PbZrO₃ and PbTiO₃. Additionally, a model for the thermal conductivity of PZT as a function of composition ($\kappa(x)$) is developed and presented. Using temperature dependent measurements of the 30/70 PZT thin film ($x = 0.7$) to extract the necessary phonon scattering constants, the resulting model agrees quite well with the experimental data for compositions $0 < x < 0.8$, yet over predicts the value of κ for compositions $0.8 < x < 1$. This discrepancy for compositions approaching $x = 1$ is due to the fact that the model does not include anharmonic phonon scattering effects, highlighting the importance of these scattering processes as the material composition approaches phase-pure PbTiO₃.

5:30 PM

(EMA-S6-010-2017) Density and size effects on the thermal conductivity of atomic layer deposition-grown amorphous alumina and titania thin films

K. E. Meyer^{*1}; B. Piercy²; M. DeCoster¹; J. Gaskins¹; M. Losego²; P. Hopkins¹; 1. University of Virginia, USA; 2. Georgia Institute of Technology, USA

We measure the room temperature thermal conductivity of atomic layer deposition-grown amorphous Al₂O₃ and TiO₂ thin films as a function of film thickness and atomic density. For films thinner than ~50 nm, we measure an effective thermal conductivity that is reduced with decreasing film thickness. This dependence is attributed to the increased influence of thermal boundary resistances as film thickness is reduced. In addition, we fit for a thickness-independent intrinsic thermal conductivity using a series-resistor model. For films thicker than ~50 nm, there is no significant dependence on thickness or substrate. We observe a strong density dependence of the thermal conductivity, which agrees well with a differential effective-medium approximation modified with a minimum limit model.

S8: Interfaces and Surfaces in Energy-Related Ceramic Materials

Effect of Interface Structure on Transport Properties

Room: Mediterranean A/B

Session Chair: Shuo Chen, University of Houston

2:00 PM

(EMA-S8-001-2017) Vertically Aligned Nanocomposite Oxide Thin Films with Enhanced Ionic Conductivity (Invited)

H. Wang^{*2}; Q. Su⁴; W. Zhang⁴; J. Huang¹; J. Jian³; C. Jacob⁵; 1. Purdue University, USA; 2. Purdue University, USA; 3. Texas A&M University, USA; 4. Texas A&M University, USA; 5. Texas A&M University, USA

Oxide thin films with high ionic conductivity are crucial for sustainable energy production systems such as fuel cells that provide efficient and environmental-friendly energy. Key materials science efforts are associated with developing such oxides with high ionic conductivity. Of particular importance for developing thin film

oxide materials is high performance and good stability in the operation temperature range. In this talk, vertically aligned nanocomposites (VAN) approach for enhancing the vertical ionic conductivity is proposed. It creates vertical interfaces of two oxide materials and provides a new design paradigm to manipulate functionalities that cannot be obtained in individual constituents. Two major examples corresponding to ionic conducting oxide thin films in the VAN form presented are: (1) vertically aligned electrolyte/electrolyte nanocomposites with superior vertical ionic conductivity, and (2) vertically aligned electrode/electrolyte nanocomposites as an interlayer to increase the catalytic reaction probability. Finally, opportunities of tuning functionalities of such VAN systems are introduced.

2:30 PM

(EMA-S8-002-2017) Three Dimensional Carbon Aerogels Infilled Membrane (3DCAM) as A New Cathode Design for Lithium Oxygen Batteries (Invited)

J. Ye^{*1}; S. Liang¹; T. Wang¹; T. Braun¹; S. Kim²; M. Biener¹; J. Biener¹;
1. Lawrence Livermore National Laboratory, USA; 2. University of Illinois at Chicago, USA

With ~10 times higher theoretical specific capacity (3505 mAh g⁻¹) and specific energy (11140 Wh kg⁻¹) compared with current Li-ion batteries, Li-O₂ batteries are considered as transformational energy sources for future electric vehicles. However, current prototype Li-O₂ batteries suffer from low power density, low energy efficiency, and poor long-term cycling stability. The main challenge of Li-O₂ battery techniques lies in the design of air-breathing cathode materials, which should be specific to their working principles. However, the start-of-the-art Li-O₂ batteries simply inherit conventional cathode designs for Li-ion batteries, which results in multiple critical issues that impede technology transfer from lab to industry. Here, we report a new cathode architecture that can tackle many of the challenges. It is based on a 3D continuous nanometer-thick ionic conducting membrane that separates the cathode into two channels: one is empty channel that allows Li⁺ transport through liquid electrolyte; the other interwoven channel is filled with porous carbon aerogels that allows fast O₂ transport through gas phase. This architecture can potentially tackle the issues including sluggish O₂ transport, O₂ cross over, solvent evaporation, and electrolyte decomposition, and consequently leads to a Li-O₂ battery with high power density and long cycling life.

3:00 PM

(EMA-S8-003-2017) Good Thermoelectric Zintl and Half-Heusler Materials (Invited)

Z. Ren^{*1}; 1. University of Houston, USA

Significant progress has been made on searching for good thermoelectric materials. Recently we have found some Zintl and half-Heusler materials have ZT higher than 1. In this talk I will discuss these materials and other related good thermoelectric materials.

Atomistic and Mesoscale Modeling of Interface Structure and Properties

Room: Mediterranean A/B

Session Chair: Ming Tang, Rice University

4:00 PM

(EMA-S8-004-2017) Modeling the Ionic Transport in Multi-Component Solid Electrolyte Interphases (SEI) in Li-ion Batteries (Invited)

Y. Qi^{*1}; 1. Michigan State University, USA

One of the significant challenges for Li-ion batteries is the control of electron and ion transport at the complex heterogeneous electrode/SEI/electrolyte interface. In this study, we predicted the ionic

transport properties in the multi-layer and multi-component SEI by developing multi-scale modeling approach and join it with experiments. We point out that the well-known two-layer structure of SEI also exhibits two different Li⁺ ion transport mechanisms. The SEI has a porous (organic) outer layer permeable to both Li⁺ and electrolyte, and a dense (inorganic) inner layer facilitate only Li⁺ transport. This model suggests a strategy to deconvolute the structure-property relationships of SEI by analyzing an idealized SEI composed of major components, such as Li₂CO₃, LiF, Li₂O, and their mixtures. After sorting out the Li⁺ ion diffusion carriers and their diffusion pathways, we design methods to accelerate the Li⁺ ion conductivity by doping and by using heterogenous structure designs. Specifically, we found that, in the ionic space charge region of Li₂CO₃ near the LiF/Li₂CO₃ interface, Li ion interstitial is accumulated but the electron is depleted. This led to an engineered nanocomposite LiF and Li₂CO₃ as an artificial SEI, in which the ionic conduction can be enhanced and the electron leakage through the SEI can be reduced.

4:30 PM

(EMA-S8-005-2017) Lattice Monte Carlo Simulation of Nucleation in Nanoparticles of Battery Intercalation Compounds

K. Yang^{*1}; M. Tang¹; 1. Rice University, USA

Many intercalation ceramic compounds for energy storage and conversion applications undergo first-order transitions upon ion insertion or extraction. An increasing number of studies show that nanoparticles of intercalation compounds exhibit significantly different phase transition behavior from their bulk counterparts, as exemplified by the extended Li solubility in nanoscale battery electrode materials. In this study we investigate the role of nucleation kinetics in rendering the unique transformation characteristics of nanoparticles through lattice Monte Carlo (LMC) simulation of nucleation process in model system lithium iron phosphate olivine, an important cathode material for Li-ion batteries. Our simulations reveal that the particle dimension dependence of critical nucleus size, Li surface exchange rate and Li diffusion anisotropy are among the important factors that control the nucleation rate in intercalation nanoparticles. Based on the comparison between LMC simulation results and the classical nucleation theory (CNT), insights are obtained on how CNT should be modified to predict nucleation kinetics in nanoscale intercalation compounds.

4:45 PM

(EMA-S8-006-2017) Design ultra-thick electrodes with multi-scale porous structure

F. Wang^{*1}; M. Tang¹; 1. Rice University, USA

In commercial lithium-ion batteries, inactive materials such as current collector and separator account for more than 50 percentage of battery weight. Realizing an order-of-magnitude increase in the electrode thickness beyond its current level will largely reduce the fraction of these inactive components and significantly enhance the overall battery energy density without changing materials chemistry. However, the severe mass transport limitation faced by ultra-thick electrodes with conventional porous structure, which results in inferior energy utilization except at very low cycling rates, represents a key bottleneck to the success of this strategy. In this work, we demonstrate through mesoscale modeling that this critical barrier can be effectively addressed by utilizing porous electrode structure with multi-scale porosity to facilitate transport kinetics. Simulations show that ultra-thick electrodes with carefully designed hierarchical microstructure can deliver much higher discharge capacity while retaining sound power performance. A new modeling methodology is proposed to efficiently optimize hierarchical porous electrodes in the design space to guide their experimental fabrication.

5:00 PM

(EMA-S8-007-2017) Solving Large-Scale Reconstructions on SrTiO₃ (111) Surfaces

T. K. Andersen^{*1}; S. U. Rahman²; L. D. Marks¹; M. R. Castell²; D. Fong³;
1. Northwestern University, USA; 2. University of Oxford, United Kingdom;
3. Argonne National Lab, USA

The surface structures of SrTiO₃, a prototypical perovskite oxide, are of interest for heterogeneous catalysis and understanding growth and nucleation of nanoparticles and thin-films. The goals of this work are determining the structure of a 5 × 5 reconstruction observed via Scanning Tunneling Microscopy (STM) on SrTiO₃ (111) using Density Functional Theory (DFT) and to test hypotheses regarding rules for structural elements of SrTiO₃ (111) reconstructions. Based on STM of a 5 × 5 SrTiO₃ (111) reconstruction, smaller unit-cell reconstructions solved on this surface, and bond-valence sum considerations candidate structures were generated. DFT calculations were performed with Wien2k, an augmented plane wave plus local orbital (APW+LO) program. As these oxides contain highly correlated electrons a hybrid functional, where a fraction of Hartree-Fock exchange is included for d-shell Ti electrons, was utilized. Resulting structures were screened, evaluated for viability based on surface energy and band gap, and re-compared to experimental data via STM simulation. The final candidates indicate there may be two symmetry-related 5 × 5 reconstructions. All solved reconstructions on SrTiO₃ (111) to date share a set of similar elements. Unsolved STM-observed reconstructions, $\sqrt{13} \times \sqrt{13}$ R13.9° and $\sqrt{7} \times \sqrt{7}$ R19.1°, offer an opportunity to explore whether these elements apply to previously uninvestigated non-integer surface unit cells.

S10: Interfacial Phenomena in Multifunctional Heterostructures: From Theory to Transport Processes

Physical and Chemical Properties of Oxide Heterostructures

Room: Caribbean B

Session Chairs: Jayakanth Ravichandran, Columbia University;
Roger De Souza, RWTH Aachen University

2:00 PM

(EMA-S10-007-2017) Evolution in Crystal Structure and Electronic Structure of Functional Oxides Probed in situ during Electrochemically Driven Phase Transition (Invited)

B. Yildiz^{*1}; Q. Lu¹; I. Massachusetts Institute of Technology, USA

Oxide systems that are conducive to phase change via control of oxygen content are potential candidate materials for non-volatile memory applications such as memristive devices. Triggering phase transition by changing oxygen content typically requires high-temperature annealing that is not practical for device applications. We have shown that applying electrochemical potential is a far more convenient way of inducing the phase transition, without changing the oxygen partial pressure (pO₂). We used epitaxial SrCoOx and VOx thin films as model systems. For SrCoOx, we found that an electrical bias of merely 30 mV was enough to trigger the phase transition from Brownmillerite (BM) phase SrCoO_{2.5} to Perovskite (P) phase SrCoO_{3-δ}. For VOx, it was possible to switch between VO₂ and V₂O₅ by applying electrochemical bias, also accompanied by a metal to semiconductor transition. We thoroughly studied the change in electronic structure of these two systems as a function of applied potential, by using in situ ambient pressure X-ray photoelectron/absorption spectroscopy (AP-XPS/XAS). We believe that these results can lay the fundamental work for using the electrochemically driven phase transition in non-volatile memory devices.

2:30 PM

(EMA-S10-008-2017) Engineering the electronic and orbital properties of the rare-earth nickelates (Invited)

C. Ahn^{*1}; 1. Yale University, USA

The interplay between the structure and physical properties of transition metal complex oxides allows for the engineering of functional properties by tuning atomic-scale structure using interfacial coupling. This principle can be applied to achieve two-dimensional electronic conductivity and orbital polarization in nickelate heterostructures. A combination of synchrotron-based experiment and first principles theory is used to identify key structural features in LaNiO₃ thin films grown using molecular beam epitaxy, allowing one to relate differences in physical structure with electronic transport properties and x-ray absorption spectroscopy measurements. By implementing design principles, such as charge transfer and inversion symmetry breaking, which lead to degeneracy breaking of the Ni 3d orbitals, one can design and fabricate tri-component superlattices to control the electronic and orbital properties of rare-earth nickelate compounds, achieving a two-dimensional single band electronic surface at the Fermi energy.

3:00 PM

(EMA-S10-009-2017) Engineering epitaxial complex oxide interfaces: From electronics to energy applications (Invited)

Y. Hikita^{*1}; 1. SLAC National Accelerator Laboratory, USA

The rich physical and chemical properties found in transition metal oxides make them essential materials for electronic and energy harvesting devices, chemical sensors, and catalysts. The capability to synthesize these oxides with atomic precision has not only provided pathways to integrate diverse physical properties at solid/solid interface, but also to apply them to solid/liquid (gas) interfaces for energy harvesting devices such as fuel cells and photocatalysts. A common challenge routinely faced in designing these interfaces is the control of carrier transport across solid/solid or solid/liquid (gas) interfaces. One powerful approach to overcome this challenge is to artificially shift the interface energy level alignments by formation of an electrostatic dipole. In this talk, I will introduce our developments toward engineering functional oxide interfaces including the control of macroscopic junction properties in all-oxide Schottky junctions and its application to oxide/liquid interfaces for solar hydrogen generation. Furthermore, I will introduce our recent development on the synthesis of a highly active oxygen evolution catalyst in acid using electrochemical processing of complex oxide epitaxial thin films.

4:00 PM

(EMA-S10-010-2017) Emerging orbital, topological, and ionic phenomena in quantum oxide heterostructures (Invited)

H. Lee^{*1}; 1. Oak Ridge National Laboratory, USA

Complex oxides are known to possess the full spectrum of fascinating properties, including magnetism, colossal magnetoresistance, superconductivity, ferroelectricity, pyroelectricity, piezoelectricity, multiferroicity, ionic conductivity, and more. This breadth of remarkable properties is the consequence of strong coupling between charge, spin, orbital, and lattice symmetry. Spurred by recent advances in the synthesis of such artificial materials at the atomic scale, the physics of oxide heterostructures containing atomically smooth layers of such correlated electron materials with abrupt interfaces is a rapidly growing area. Thus, we use pulsed laser epitaxy to assemble the building blocks to a functional system, yielding many intriguing physical properties that cannot be found in bulk counterparts. In this talk, examples of functional interfaces will be presented, highlighting the importance of heterostructuring, interfacing, and straining. The main topics include (1) strain control of orbital polarization in LaNiO₃ thin films for improved oxygen catalysis, (2) anomalous Hall effect discovered in 3d-5d oxide heterostructures, and (3) high oxygen ion conductivity found at interfaces in CeO₂-based nanosuperlattices. *This

work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

4:30 PM

(EMA-S10-011-2017) Affecting point defects in perovskite-type oxides by voltage, light and dislocations (Invited)

J. Fleig^{*1}; 1. TU Wien, Austria

The equilibrium bulk defect chemistry of many oxides is rather well understood. However, materials in real (multi-)functional devices are often far from equilibrium. Driving forces for non-equilibrium situations include applied voltages, irradiation by light and structural non-idealities such as dislocations. This is illustrated by several examples with novel findings on perovskite-type thin films and bulk samples. i) In (La,Sr)MnO₃ (LSM) thin films grain boundaries and dislocations lead to accelerated oxide ion transport. Together with voltage induced defect concentration gradients this causes apparent uphill diffusion of ¹⁸O tracer ions. ii) SrTiO₃ thin films exhibit electronic and ionic charge transport properties that differ strongly from those of bulk material. This is most probably related to space charges along extended defects. The properties can be further affected by voltages and defect motion manifests itself in scan-rate dependent I-V curves. iii) Heterostructures of SrTiO₃ with other oxides show novel UV light induced high temperature effects: (La,Sr)CrO₃ on a SrTiO₃ single crystal results in a solar cell with OCV of 900 mV at 400°C and SrTiO₃ on yttria stabilized zirconia (YSZ) leads to an electrochemical cell which can be charged by light. The latter is caused by oxygen uptake of SrTiO₃ under illumination.

5:00 PM

(EMA-S10-012-2017) Tunable Nanionics in Epitaxial Oxide Nanocomposite Thin Films (Invited)

J. MacManus-Driscoll^{*1}; S. Cho¹; C. Yun¹; S. Lee²; R. Wu¹; A. Kursomovic¹; 1. University of Cambridge, United Kingdom; 2. Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea

The strong interplay of structural, electronic and magnetic degrees of freedom in correlated oxides are important for realizing novel multifunctional properties. In recent years the ionic degree of freedom has also been widely explored and the discovery of nanionic memristive effects in oxide thin films has sparked off research activities towards a universal device involving terabit memories, logic operators, neuristors, and nanobatteries. In this work, we show that it is possible to nanoengineer ionic channels into films using vertical nanocomposite structures. The ionic channels can act as fast ionic diffusion channels and can also as electron trapping sites. The extent of ionic versus electronic conductivity can be tuned by appropriate selection of phases in the composites and the strain levels in the system.

5:30 PM

(EMA-S10-013-2017) Properties of the conducting LaInO₃/BaSnO₃ polar interface (Invited)

K. Char^{*1}; 1. Seoul National University, Republic of Korea

We have recently reported on the conducting LaInO₃/BaSnO₃ polar interface. We have found that a small amount of doping in the BaSnO₃ layer is critical for the conducting behavior, while the interface between the LaInO₃ and the undoped BaSnO₃ was not conducting. By way of series of experiments, we show that the conducting behavior is due to neither oxygen vacancies nor cation diffusion at the interface. One of such experiments is a modulation doped heterostructure, where an undoped BaSnO₃ spacer layer is inserted between the LaInO₃ and the slightly doped BaSnO₃. We will report on the electrical properties of such structures. We will also report on the properties of the BaSnO₃ interface with other larger bandgap perovskite materials, including nonpolar BaHfO₃ and SrZrO₃ epitaxial perovskites. Our model for the conducting interface is based on the 2DEG-like structure created by interface polarization

of the LaInO₃ and the Fermi level controlled by the doping in the BaSnO₃. Using such LaInO₃/BaSnO₃ conducting interfaces, all perovskite transparent FETs with excellent properties were made. We believe that the stable oxygen stoichiometry and the ability to control the local doping level in LaInO₃/BaSnO₃ heterostructures will lead to understanding of the 2DEG behavior, tuning the carrier density, creating high density 2DEG, and eventually further increasing the high carrier density and the mobility.

6:00 PM

(EMA-S10-027-2017) Emergence of room-temperature ferroelectricity at reduced dimensions (Invited)

D. Lee^{*1}; H. Lu²; Y. Gu³; S. Choi⁴; S. Li⁵; S. Ryu¹; T. Paudel²; K. Song⁶; E. Mikheev⁷; S. Lee¹; S. Stemmer⁷; D. Tenne⁸; S. Oh⁶; E. Tsybal²; X. Wu⁵; L. Chen³; A. Gruverman²; C. Eom¹; 1. University of Wisconsin-Madison, USA; 2. University of Nebraska-Lincoln, USA; 3. Pennsylvania State University, USA; 4. Korea Institute of Materials Science, Republic of Korea; 5. Temple University, USA; 6. Pohang University of Science and Technology (POSTECH), Republic of Korea; 7. University of California-Santa Barbara, USA; 8. Boise State University, USA

The enhancement of the functional properties of materials at reduced dimensions is crucial for continuous advancements in nanoelectronic applications. Here, we report that the scale reduction leads to the emergence of an important functional property, ferroelectricity, challenging the long-standing notion that ferroelectricity is inevitably suppressed at the scale of a few nanometers. A combination of theoretical calculations, electrical measurements, and structural analyses provides evidence of room-temperature ferroelectricity in strain-free epitaxial nanometer-thick films of otherwise nonferroelectric strontium titanate (SrTiO₃). We show that interfacial charge compensation for naturally existing polar nanoregions is responsible for the appearance of a stable net ferroelectric polarization in these films. This finding can be useful for the development of low-dimensional material systems with enhanced functional properties relevant to emerging nanoelectronic devices.

S14: Multifunctional Nanocomposites

Multifunctional Nanocomposites: Functionality by Design III

Room: Caribbean C

Session Chair: Bryan Huey, University of Connecticut

2:00 PM

(EMA-S14-022-2017) Monolithic integration of room-temperature multifunctional BaTiO₃-CoFe₂O₄ epitaxial heterostructures on Si(001) (Invited)

M. Scigaj¹; N. Dix¹; J. Gazquez¹; M. Varela²; I. Fina¹; N. Domingo³; G. Herranz¹; V. Skumryev⁴; J. Fontcuberta¹; F. Sanchez^{*1}; 1. Institut de Materials Science of Barcelona (ICMAB-CSIC), Spain; 2. Universidad Complutense, Spain; 3. ICN2, Spain; 4. ICREA, Spain

The multifunctional response at room temperature that is elusive in single phase multiferroic materials can be achieved in a proper combination of ferroelectric perovskites and ferrimagnetic spinel oxides in horizontal heterostructures. However, perovskites and spinels are highly dissimilar, which hinders epitaxial growth in horizontal heterostructures. We will show that using suitable deposition conditions CoFe₂O₄/BaTiO₃ epitaxial bilayers can be grown with excellent properties, even on silicon wafers. The growth is more difficult on silicon wafers than on oxide substrates because the c-axis of BaTiO₃ tends to be in the plane due to the tensile stress caused by the thermal mismatch between BaTiO₃ and Si. To permit epitaxial growth and reduce thermal mismatch effects we have integrated lead-free CoFe₂O₄/BaTiO₃ multiferroic bilayers with Si(001) using LaNiO₃/CeO₂/YSZ as a tri-layer buffer. The bilayers present properties close to those achieved on perovskite substrates.

They are very flat and epitaxial, presenting c-oriented BTO with an expanded c-axis. The bilayers show multifunctional properties at room temperature, with magnetization above 200 emu/cm³, remnant polarization higher than 20 $\mu\text{C}/\text{cm}^2$, high endurance and low leakage. These artificial multiferroics are thus potential candidates for non-volatile four states multiferroic monolithic memories.

2:30 PM

(EMA-S14-023-2017) Ultrafast control of ferroelectric states by intense terahertz field pulses (Invited)

H. Wen^{*1}; 1. Argonne National Lab, USA

An ultrafast electric field that turns on and off within 1 picosecond in a form of an intense broadband terahertz pulse provide a new means to manipulate ferroelectric states in a non-contact fashion. In this talk, I will present time-resolved studies on prototypical ferroelectrics BaTiO₃ (BTO) and a novel ferroelectric vortex state in PbTiO₃/SrTiO₃ (PTO/STO) superlattices using THz pump, hard x-ray probe capability at large-scale x-ray facilities. The intrinsic structural responses of ferroelectric materials are revealed upon intense THz excitation, showing an ultrafast rotation of ferroelectric polarization in BTO and ultrafast conversion and recovery of vortex and a1/a2 domain structures in PTO/STO superlattice. In addition, we demonstrate that the near-field THz excitation assisted by meta-surfaces and ultrafast x-ray diffraction imaging open new opportunities of transient spatial engineering of complex materials. This work is supported by the U.S Department of Energy, Office of Science, Office of Basic Energy Sciences.

3:00 PM

(EMA-S14-024-2017) Quasi 2D oxide composite skins for autonomous systems (Invited)

S. Ramanathan^{*1}; 1. Purdue University, USA

Much as the 20th century saw the evolution of solid state devices for information processing, an early stage field seeing rapid growth is autonomous systems and humanoid interfaces. Oxide ion and electron conductors could have much to contribute to these topics. I will discuss overarching problems concerning the role of new multi-functional materials in miniature autonomous systems and evolving devices. Subsequently, I will present collaborative results on ion conducting oxide composites and heterostructure membranes monolithically integrated onto miniature robot exoskeletons for power generation and sensing. Fundamental problems that will be emphasized include understanding thermo-mechanical stresses involving suspended oxide membranes and their connection to ionic conduction, in-situ visualization of actuation dynamics. Innovative materials synthesis plays a major role in these efforts, since deposition and annealing temperatures as well as stress states must be kept compatible with structural and chemical stability of structural features. The use of quasi-2D oxides as symbiotic skins then opens up the problem of understanding electrostatics and carrier inversion at interfaces under extreme chemical gradients, a fledgling field that would benefit from cross-disciplinary interactions.

Multifunctional Nanocomposites: The Interface II

Room: Caribbean C

Session Chair: Xia Hong, University of Nebraska-Lincoln

4:00 PM

(EMA-S14-025-2017) Understanding oxygen vacancies formed in 1D oxide nano-superlattices

X. Gao^{*1}; D. Lee¹; M. F. Chisholm¹; H. Lee¹; 1. Oak Ridge National Laboratory, USA

Nanostructures offering the physical properties superior to their bulk counterparts and the ability to synthesize such functional nanomaterials are critical to advance information and energy technologies. We recently developed a synthesis technique to grow vertically oriented, highly porous 1D nanostructures by pulsed laser

epitaxy. In particular, we found colossal ionic conductivity in the interfacial 1D nanostructure. By utilizing state-of-the-art scanning transmission electron microscopy (STEM), we have investigated the origin of the highly enhanced ion conduction focusing on the local atom structure, chemical bonding, and strain states of the 1D oxide superlattices composed of CeO₂ based binary oxides epitaxially grown on YSZ substrates. Angle-resolved STEM imaging and electron energy-loss spectroscopy (EELS) analysis reveal a unique lattice strain field, associated with the creation of a high number of oxygen defects. In the presentation, results on microstructural evolution to form the nano-superlattice structure as well as reasons for the formation of oxygen vacancies and lattice strain will be discussed. *This work was supported by the U.S. Department of Energy, Office of science, Basic Energy Sciences, Materials Sciences and Engineering Division.

4:15 PM

(EMA-S14-026-2017) Conducting interface in oxide homojunction: Understanding of superior properties in black TiO₂ (Invited)

X. Lu^{*1}; A. Chen¹; P. Lu²; E. Enriquez¹; H. Xu¹; Q. Jia³; 1. Los Alamos National Lab, USA; 2. Sandia National Laboratories, USA; 3. University at Buffalo, USA

Extraordinary emergent properties have been generated at interfaces between oxides, including interfacial superconductivity and high-mobility electron gases. Here, we have fabricated oxide homojunction films with enhanced electronic properties and the underlying mechanism has been revealed. Specifically, TiO₂ composite films consisting of an oxygen-deficient amorphous layer on top of a highly crystalline layer were grown by pulsed laser deposition. Metallic conduction is achieved at the crystalline-amorphous homointerface via electronic interface reconstruction, which is the major mechanism responsible for the enhanced electron conduction of black TiO₂, a promising material for energy purposes. This work not only achieves an unprecedented understanding of black TiO₂, but also provides a new perspective for investigating carrier generation and transport behavior at oxide interfaces, which are of tremendous fundamental and technological interest.

4:30 PM

(EMA-S14-028-2017) Enhanced Magnetic Properties and Spin-Seebeck Effect in Epitaxial Nickel Ferrite Thin Films and Heterostructures (Invited)

A. Gupta^{*1}; 1. University of Alabama, USA

Ferrite thin films are promising candidates for future spintronic devices. However, spinel ferrite thin films such as NiFe₂O₄ (NFO) suffer from a number of structural and magnetic drawbacks, e.g. formation of antiphase boundaries and high magnetic saturation fields. We show that by using substrates having similar crystal structure and low lattice mismatch, one can avoid formation of antiphase boundaries and thereby obtain magnetic properties comparable to bulk. We used spinel MgGa₂O₄ and CoGa₂O₄ substrates, which have 0.8% and 0.2% lattice mismatch, respectively, with NFO to grow films that are free of antiphase boundaries and exhibit sharp magnetic hysteresis characteristics. Moreover, ferromagnetic resonance linewidths similar to those in single crystals are obtained. We have compared these results with NFO film grown on another spinel substrate MgAl₂O₄, which has 3.1% lattice mismatch, that has antiphase boundaries and clearly exhibits degraded properties. We also investigated spin transport properties in the films grown on the three substrates via the longitudinal spin Seebeck effect (LSSE). An increase in the spin voltage signal with reduction in lattice mismatch is observed, which is in correspondence with similar improvements in structural and magnetic properties. We also studied the LSSE in heterostructures of NFO with antiferromagnetic NiO.

5:00 PM

(EMA-S14-029-2017) Enhanced Energy Density with Wide Thermal Stability in Epitaxial $\text{Pb}_{0.92}\text{La}_{0.08}\text{Zr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ Thin Films

C. Ma^{*1}; G. Hu¹; W. Wei¹; Z. Sun¹; L. Lu¹; S. Mi¹; M. Liu¹; B. Ma³; J. Wu²; C. Jia¹; 1. Xi'an Jiaotong University, China; 2. University of Kansas, USA; 3. Argonne National Lab, USA

High-quality epitaxial $\text{Pb}_{0.92}\text{La}_{0.08}\text{Zr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ (PLZT) films of thickness of ~880 nm were fabricated using pulsed laser deposition on (001) Nb doped SrTiO_3 (Nb:STO) substrates. Besides a confirmation of the epitaxial relationship $[100]_{\text{PLZT}} // [100]_{\text{Nb:STO}}$ and $(001)_{\text{PLZT}} // (001)_{\text{Nb:STO}}$ using X-ray diffraction, a transmission electron microscopy study has revealed a columnar structure across the film thickness. The recoverable energy density (W_{rec}) of the epitaxial PLZT thin film capacitors increases linearly with the applied electric field and the best value of ~31 J/cm³ observed at 2.27 MV/cm is considerably higher by 41% than that of the polycrystalline PLZT film of a comparable thickness. In addition to the high W_{rec} value, an excellent thermal stability as illustrated in a negligible temperature dependence of the W_{rec} in the temperature range from room temperature to 180°C is achieved. The enhanced W_{rec} and the thermal stability are attributed to the reduced defects and grain boundaries in epitaxial PLZT thin films, making them promising for energy storage applications that require both high energy density, power density and wide operation temperatures.

5:15 PM

(EMA-S14-030-2017) A radial-quadrant domain structure in ferroelectric nanoplates: A new route into charged domain walls and topological structures (Invited)

C. Yang^{*1}; 1. KAIST, Republic of Korea

Nanoscale electronic conduction in ferroelectric materials has attracted a lot of attention because of their potential applications in nano-electronic devices. Controllable switching between n- and p-type conduction has been suggested by arranging two opponent polarizations in a head to head (or tail to tail) configuration. However, such charged domain walls have been rarely observed because of their unstable electrostatic energy. Here, we report that nanoscale ferroelectric plates imbedded in other matrix materials can provide a new promising opportunity into creation of charged domain walls because of their highly anisotropic mechanical boundary condition. We demonstrate a ferroelectric nanoplate exhibits an exotic radial-quadrant in-plane ferroelectric domain structure at the merging point of which electronic conduction is significantly enhanced. A large strain gradient plays a critical role in the emergence of unusual ferroelectric/ferroelastic domain configurations each of which has a unique topological number.

S15: Superconducting Materials and Applications**Characterization of Structural, Magnetic, and Superconducting Properties**

Room: Pacific

Session Chairs: Hai-Hu Wen, Nanjing University; Sergey Bud'ko, Ames Laboratory / Iowa State University

2:00 PM

(EMA-S15-019-2017) Electronic Structure and Superconductivity of FeSe-Related Superconductors (Invited)

X. Zhou^{*1}; 1. Chinese Academy of Sciences, China

In this talk, I will report high-resolution angle-resolved photoemission measurements on the electronic structure and superconducting gap of an FeSe-based superconductor, $(\text{Li}_{0.84}\text{Fe}_{0.16})\text{OHFeSe}$, with a T_c at 41 K [1]. We find that this single-phase bulk superconductor shows remarkably similar electronic behaviors to that of the

superconducting single-layer FeSe/ SrTiO_3 films[2,3] in terms of Fermi surface topology, band structure and the gap symmetry. These observations provide new insights in understanding high-temperature superconductivity in the single-layer FeSe/ SrTiO_3 films and the mechanism of superconductivity in the bulk iron-based superconductors. Some other latest results on FeSe/ SrTiO_3 films will also be presented and implications will be discussed. [1].Lin Zhao, Aiji Liang, Dongna Yuan, Yong Hu, Xiaoli Dong and X. J. Zhou et al., Nature Communications 7, 10608 (2016); [2].Defa Liu, Wenhao Zhang, Daixiang Mou, Junfeng He, Xucun Ma, Qikun Xue and X. J. Zhou et al., Nature Communications 3, 931 (2012); [3].Shaolong He, Junfeng He, Wenhao Zhang, Lin Zhao, Xucun Ma, Qikun Xue and X. J. Zhou et al., Nature Materials 12, 605 (2013).

2:30 PM

(EMA-S15-020-2017) Charge Doping and Magneto-structural Effects in Iron-based Superconductors (Invited)

A. S. Sefat^{*1}; 1. Oak Ridge National Laboratory, USA

The chemical, magnetic, and electronic states coexisting and competing in a material controls the superconducting state and value of critical transition temperature. In this talk, I will review some of our recent experimental investigation on the effects of charge doping and magneto-structural effects in barium iron arsenide, with theoretical input. Recent ORNL findings include the following: (a) Sufficiently strong magnetoelastic coupling in thallium-doped BaFe_2As_2 reverses the usual trend of diminished Néel temperature with charge doping [1]; (b) Effects of disorder in large nematic region and filamentary superconductivity in gold-doped BaFe_2As_2 [2]; (c) Persistent magnetism and strong electronic scattering in silver-doped BaFe_2As_2 [3]. This work was primarily supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

3:00 PM

(EMA-S15-021-2017) Microscopic Nature of High- T_c Superconductivity in Interfacial FeSe at Strong $e^- - e^-$ Repulsion (Invited)

J. P. Rodriguez^{*1}; 1. California State University at Los Angeles, USA

Heavily electron-doped surface layers of FeSe have reached critical temperatures for the onset of superconductivity in excess of 100 K. It is important to uncover the microscopic symmetry of the Cooper pairs in order to predict effective pinning centers. We describe the electronic structure of a single layer of electron-doped FeSe by a local-moment model at strong on-site electron-electron repulsion. At small electron doping and moderately strong Hund's Rule coupling, mean field plus exact numerical calculations of the low-energy spectrum find electron-type Fermi-surface pockets at the corners of the Brillouin zone and hole bands that lie buried below the Fermi level at the center of the Brillouin zone. These results agree roughly with the electronic structure in heavily electron-doped FeSe determined by angle-resolved photoemission spectroscopy (ARPES). Exact numerical calculations for a single Cooper pair of mobile electrons find an isotropic S-wave groundstate that alternates in sign between the electron Fermi surface pockets at the corners of the Brillouin zone and the buried hole bands at the center of the Brillouin zone. The latter pairing is therefore remnant. We explore what types of defects make good pinning centers in such remnant S^+ superconductivity.

4:00 PM

(EMA-S15-022-2017) A BCS-like model for heavy fermion superconductivity (Invited)

Y. Yang^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

Unconventional superconductivity in correlated electron systems such as cuprates and heavy fermions shares many similarities. In particular, its interplay with magnetism may be traced back to the dual (simultaneously localized and itinerant) behavior of strongly

correlated electrons that has been experimentally established in both superconductors. Itinerant quasiparticles coexist with interacting local moments out of which they are born, leading to a phenomenological two-fluid description of the correlated electrons. The spin interaction is therefore expected to set the fundamental energy scale for the superconductivity. In this talk, I will extend a simple spin-fluctuation model previously developed for cuprate superconductors and combine it with the unusual dual behavior of the f-electrons to propose a simple BCS-like model for heavy fermion superconductivity. I will show that our simple model provides a quantitative explanation of the pressure-dependent T_c in the “hydrogen atoms” of unconventional superconductivity, CeCoIn_5 and CeRhIn_5 , and its coexistence with long-range antiferromagnetic order. I will then apply the model to CeCu_2Si_2 and discuss its implication on its mysterious superconducting gap symmetry.

4:30 PM

(EMA-S15-023-2017) Interplay between magnetism, structure, and superconductivity in Mo_3Sb_7 (Invited)

J. Yan^{*1}; 1. Oak Ridge National Lab, USA

Despite a relatively low superconducting transition temperature $T_c = 2.08$ K, the Zintl compound Mo_3Sb_7 has attracted much interest due to the possible involvement of magnetism in superconducting pairing, and promising thermoelectric performance with proper doping. Mo_3Sb_7 crystallizes in Ir_3Ge_7 -type cubic structure with space group $\text{Im}\bar{3}\text{m}$ at room temperature. A structure transition from cubic to tetragonal (I4/mmm) was observed at $T_{\text{str}} = 53$ K and this symmetry lowering is accompanied by the opening of a 120 K spin gap. Mo_3Sb_7 thus provides an interesting platform to study the interplay between a structural anomaly, magnetism, and superconductivity. In this talk, I will present the intrinsic physical properties of Mo_3Sb_7 and how chemical doping and hydrostatic pressure disturb the complex interplay between structure, magnetism, and superconductivity. The role of magnetism will be discussed based on thermal conductivity change across T_c and the pressure/doping dependence of T_c and T_{str} . Work at ORNL was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

5:00 PM

(EMA-S15-024-2017) Understanding doping, vacancy, lattice stability, and superconductivity in $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$

G. Wang^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

$\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ and its derivatives differ from other superconductors in the existence of iron vacancy, potassium contents and phase separation, which result in no consensus on the phases responsible for the observed superconductivity at 30 ~ 46 K has been reached. Here, we put forward a unified scenario based on the study of structural stability and lattice dynamics in terms of the intercalated K, which allows us to understand the structural evolution and identify the superconducting phases. It is found that the intercalated K contents between FeSe layers determine the formation energy, structural stability, and the driving force for the appearance of Fe vacancies. The underlying mechanism is that intercalated K alters the Coulomb attraction between K ions and FeSe layers and the energy due to the accumulation of negative charge in FeSe layers. A phase diagram is constructed for showing the structural evolution of this series of phases in terms of K-intercalated levels x . The superconductors are determined to be $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ with $0.25 \leq x \leq 0.6$ and $y \approx 0$, in which their transition temperatures rely on x . We believe that these findings should also apply to other metal-intercalated iron selenides.

5:15 PM

(EMA-S15-025-2017) The synthesis and physical properties of new layered oxyhalides

T. Kitamura^{*1}; 1. The University of Tokyo, Japan

Layered mixed anion compounds have attracted considerable attention due to the wide variety of electronic and magnetic behaviors such as superconductivity, thermoelectricity and colossal magnetoresistance. The recent discovery of Fe-based superconductor REFeAsO ($\text{RE} = \text{La} \sim \text{Tb}$), has stimulated extensive research for mixed anion systems. Recently, a new BiS_2 -based superconductor, $\text{Bi}_2(\text{O,F})\text{S}_2$ with $T_c = 5.1$ K was discovered in our group. $\text{Bi}_2(\text{O,F})\text{S}_2$ was obtained as the main phase by topotactic fluorination of undoped Bi_2OS_2 using XeF_2 . Topotactic reaction enables kinetically unstable phases to be synthesized through anion substitution, and the substitution of F⁻ by O^{2-} in the oxide blocks induces superconductivity via electron doping in this compound. In this study, synthesis and physical properties of new oxyhalide $\text{Sr}_2\text{RuO}_3\text{F}_2$ are reported. $\text{Sr}_2\text{RuO}_3\text{F}_2$ was successfully synthesized by topotactic fluorination of Sr_2RuO_4 with fluorinating agents such as ZnF_2 , CuF_2 and PVDF. Since fluorine substitution and insertion into interstitial sites are expected in this reaction, the valence state of Ru does not change after the reaction. $\text{Sr}_2\text{RuO}_3\text{F}_2$ showed paramagnetic and semiconductor behavior. Further investigation into $\text{Sr}_2\text{RuO}_3\text{F}_2$ and the attempt of the synthesis of other oxyhalides are also reported in the presentation.

5:30 PM

(EMA-S15-026-2017) Development of high performance $\text{SmFeAs}(\text{O,F})$ superconductor

K. Hayashi^{*1}; H. Ogino²; J. Shimoyama³; K. Kishio¹; 1. University of Tokyo, Japan; 2. National Institute of Advanced Industrial Science and Technology (AIST), Japan; 3. Aoyama Gakuin University, Japan

$\text{SmFeAs}(\text{O,F})$ [Sm1111], which have the highest $T_c = 55$ K among the iron-based superconductors, have been intensively studied for practical applications. It is reported that Sm1111 synthesized at low sintering temperature with slow cooling rate has high T_c because of its high fluorine doping level. Furthermore, the addition of Sn to Sm1111 increase intergranular critical current density J_c without decreasing T_c . In this study, optimization of synthesis condition of Sn added Sm1111 were attempted. In addition, synthesis with short sintering time was applied to investigate the Sn addition effect. All samples were prepared by the solid-state reaction. To develop high performance Sm1111 superconductor, low-temperature synthesis and the Sn addition were combined, and intergranular J_c was improved by sintering for long time and re-sintering. To confirm the effect of Sn addition, Sn-added Sm1111 samples were synthesized at 900°C for 1, 5, 15 h with rapid cooling process. Sm1111 was obtained as main phase even at sintering time of 1 h, and their constituent phase didn't change, while a lattice parameter became smaller and their $T_{c\text{onset}}$ increased with increasing sintering time. Microstructural analysis revealed that Sm1111 regions around Sn metal became larger with increasing sintering time, indicating that Sm1111 regions around Sn metal become denser after formation of Sm1111 .

Friday, January 20, 2017

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Energy Storage, Conversion, and Harvesting Materials and Device Structures I

Room: Indian

Session Chair: Rudeger Wilke, Sandia National Laboratories

8:30 AM

(EMA-S1-036-2017) Impact of phase transition sequence on the electrocaloric effect in PbZrO₃-based ceramics

Z. Xu¹; Z. Fan¹; X. Tan^{*1}; 1. Iowa State Univ, USA

The electrocaloric effect describes the temperature change when an electric field is applied or removed from a material under adiabatic conditions. PbZrO₃-based compositions have been shown to exhibit large electrocaloric effect in the vicinity of their phase transition temperatures. The requirement of intense applied electric fields has limited most studies to materials in the thin film form. The present work focuses on bulk ceramics of chemically modified PbZrO₃ compositions. Two compositions with opposite phase transition sequences are comparatively investigated. When temperature increases, the first composition transforms from a ferroelectric phase to an antiferroelectric phase, while the second composition changes from an antiferroelectric to a ferroelectric phase. From the indirect measurements, it is found that the first composition displays a normal electrocaloric effect. In contrast, the second composition exhibits a negative electrocaloric effect of $\Delta T \approx -4\text{K}$ at a moderate electric field of 130 kV/cm. The negative effect is attributed to the existence of the ferroelectric phase at higher temperatures than the antiferroelectric phase, producing a positive temperature coefficient of polarization evolution close to the phase transition.

8:45 AM

(EMA-S1-037-2017) Ferroelectric enhancement, band-gap engineering and photovoltaic response of the ternary system: PbTiO₃-BiFeO₃-Bi(Ni_{1/2}Ti_{1/2})O₃

L. Wu^{*1}; D. Imbrenda²; A. A. Podpirka³; J. E. Spanier³; P. K. Davies¹; 1. University of Pennsylvania, USA; 2. Drexel University, USA; 3. Drexel University, USA

Ferroelectrics can exhibit the bulk photovoltaic effect (BPE) which fundamentally differs from a conventional p-n junction. Features of BPE, such as large open-circuit voltage and potentially high efficiency, make semiconducting ferroelectrics promising in photovoltaic applications. Large remnant polarization and narrow band-gap are believed to be crucial to improve photovoltaic performance, while very few ferroelectric ceramics possess both of them. Here we demonstrate the design of a ternary compound (1-x)[(1-y)PbTiO₃-yBiFeO₃]-xBi(Ni_{1/2}Ti_{1/2})O₃ which exhibits large bulk polarization and narrow bandgap simultaneously. BiFeO₃ is found to be effective to lower the bandgap of PbTiO₃ from 3.2 eV to ~2.2 eV and enhance its tetragonality to $c/a = 1.17$. Bi(Ni_{1/2}Ti_{1/2})O₃ dopant further reduces the bandgap of end-member (1-y)PbTiO₃-yBiFeO₃ and also introduces a morphotropic phase boundary (MPB) which leads to enhanced ferroelectric properties. Phase diagrams which reveal the band-gap evolution and MPB regions of the ternary system will be presented. MPB compositions of $x = 0.4$, $y = 0.3$ ($P_r = 41 \mu\text{C}/\text{cm}^2$, $E_g \approx 2.4 \text{ eV}$) and $x = 0.22$, $y = 0.5$ ($P_r = 31 \mu\text{C}/\text{cm}^2$, $E_g \approx 2.3 \text{ eV}$) are further characterized by their photovoltaic responses. These results demonstrate a novel route to integrate multifunctionalities through careful control of their bulk chemical composition.

9:00 AM

(EMA-S1-038-2017) Design of Multilayer Ferroelectrics for Pyroelectric Energy Conversion

Y. Espinal^{*1}; P. S. Alpay¹; R. G. Polcawich²; B. Hanrahan²; 1. University of Connecticut, USA; 2. US Army Research Laboratory, USA

Using ferroelectric materials for pyroelectric energy conversion shows promise for waste heat recovery. Our theoretical results show that the dielectric and pyroelectric properties of monodomain ferroelectric films can be optimized using linear dielectric buffer layers interposed between metallic electrodes. Here, we will first provide a quantitative computational analysis for multilayers consisting of PbZr_{0.3}Ti_{0.7}O₃ with Al₂O₃, SiO₂, Si₃N₄, HfO₂ and TiO₂ buffers on metalized Si. In an effort to experimentally support these theoretical results we have prepared 500 nm-thick PbZr_{0.3}Ti_{0.7}O₃ films with thin (< 25nm) Al₂O₃ and HfO₂ buffer layers sandwiched between platinum electrodes on a silicon substrate. The heterostructures were structurally characterized with XRD and cross-sectional SEM. Temperature-dependent pyroelectric, dielectric, and leakage current responses were measured from 20-200°C. The device figure of merit was determined for the tested material systems and results were compared to predictions from theory. The results show that such constructs could potentially provide significant performance advantages for pyroelectric energy conversion applications.

Energy Storage, Conversion, and Harvesting Materials and Device Structures II

Room: Indian

Session Chairs: Sean Garner, Corning Incorporated; Chun-Ming Wang, Shandong University

10:00 AM

(EMA-S1-039-2017) Ultra-Slim Flexible Glass for Optical and Electronic Applications (Invited)

S. Garner^{*1}; 1. Corning Incorporated, USA

As optical and electronic devices evolve to become lighter, thinner, and more flexible, the substrate choice continues to be critical to their overall optimization. The substrate directly affects improvements in the designs, materials, fabrication processes, and performance of advanced electronics. With their inherent benefits such as surface quality, optical transmission, hermeticity, and thermal and dimensional stability, glass substrates enable high-quality and long-life devices. As substrate thicknesses are reduced below 200µm, ultra-slim flexible glass continues to provide these inherent benefits to high-performance flexible devices. In addition, the reduction in glass thickness also allows for new device designs and high-throughput, continuous manufacturing enabled by roll-to-roll processes. This paper provides an overview of flexible glass substrates and how they enable optical and electronic device optimization. Also included is the most recent information related to flexible glass R2R conveyance and device fabrication.

10:30 AM

(EMA-S1-040-2017) Unusual electrical properties and piezoresponse studies of antiferroelectric sodium niobate (NaNbO₃) (Invited)

C. Wang^{*1}; 1. Shandong University, China

Antiferroelectrics (AFEs) are important materials for applications in transducers, energy storage capacitors, and electrocaloric cooling devices. Sodium niobate (NaNbO₃), a typical AFE compound, has draw extensive attention as lead-free alternative to PZT. However, the macroscopic and local electrical properties as well sintering characteristics are not sufficiently understood. In this work, we have successfully fabricated high-density NaNbO₃ with cubic-shaped grains, presenting a very low dielectric loss $\tan \delta < 1\%$. The poled NaNbO₃ exhibits saturated hysteresis loops with remnant polarization of 13.9 mC/cm² and desirable piezoelectric coefficient

d_{33} of 50 pC/N. The local domain switching behaviors were studied. The as-polished NaNbO_3 exhibit very weak domain patterns, but further piezoresponse hysteresis loops measurements show that the typical reversible loops can be obtained under switching voltages. The tip-voltage-poled NaNbO_3 shows quite unusual domain configurations responsible for ferroelectric behaviours. The above observations clearly demonstrated that NaNbO_3 can be locally transformed from antiferroelectric to ferroelectric at strong dc electric field.

11:00 AM

(EMA-S1-041-2017) Reduced temperature sensitivity of relative permittivity in dipole-like substituted BaTiO_3 for high-temperature capacitor technology

V. Kaliyaperumal Veerapandian^{*1}; W. Schulze¹; S. Mixture¹; S. Pilgrim¹; D. M. Potrepka²; F. Crowne²; A. Tauber³; S. C. Tidrow¹; 1. Kazuo Inamori School of Engineering, Alfred University, USA; 2. U.S. Army Research Laboratory, Sensors Electron Devices Directorate, USA; 3. As contracted to the U. S. Army Research Laboratory from Geo-Centers Inc.; presently retired, USA

$\text{Ba}_{(1-x)}\text{Sr}_x[\{\text{Ga}_y, \text{Ta}_y\}\text{Ti}_{(1-2y)}]\text{O}_3$ materials with (x,y) values of (0.8, 0), (0.8, 0.05), (0, 0), and (0, 0.05) were investigated to understand the effect of dipole-like substitutions ($y > 0$) on the dielectric properties of the solid-solution Barium-Strontium-Titanate ($\text{Ba}_{(1-x)}\text{Sr}_x\text{TiO}_3$). The dipole-like substitution on the B-site of the ABO_3 perovskite results in significant reduction in the temperature sensitivity of the material capacitance through flattening of the relative permittivity (ϵ_r) curve. Dielectric measurements as a function of temperature [-100°C, 800°C] reveal changes in Curie temperature and Curie constant. In-situ XRD, including use of Rietveld refinement have been performed to determine the lattice parameters, coefficient of thermal expansion and phase transition temperature(s) over the temperature range [RT, 1000°C]. $\text{Ba}[(\text{Ga}_{0.05}, \text{Ta}_{0.05})\text{Ti}_{0.9}]\text{O}_3$ presents a flat ϵ_r curve with a ϵ_r value of $\sim 700 \pm 16\%$ and dissipation factor < 0.1 at 10 kHz over the temperature range [-75°C, 120°C]. Combinations of A-site and B-site substitutions are explored in an attempt to increase the capacitance, and extend the temperature range of capacitance operation while maintaining the trend of temperature insensitive relative permittivity.

11:15 AM

(EMA-S1-042-2017) Polymeric Bonding of Alkali-Free Glass to form Multi-Layer Capacitors

R. Wilke^{*1}; H. Brown-Shaklee¹; A. Casias³; R. Johnson-Wilke¹; M. Vecchio²; B. Cunningham³; R. Vudatha¹; 1. Sandia National Laboratories, USA; 2. Pennsylvania State University, USA; 3. Sandia National Laboratories, USA; 4. Cornell University, USA

Alkali-free glasses show immense promise as a potential high dielectric energy density storage material. Commercially available alumino-borosilicate compositions exhibit high breakdown strengths (exceeding 1000 MV/m), low loss ($\tan \delta < 0.01$), modest relative permittivities (5-7), and high dielectric energy storage densities (35 J/cc). In order to take advantage of the intrinsic properties of these materials it is necessary to develop processing and packaging strategies for fabricating devices with appreciable capacitance values. We have fabricated multi-layer devices using Epon 828/Jeffamine T403 to bond individually processed sheets of glass. The thickness of this layer is controlled by bonding under uniaxial pressure. The capacitors are then fabricated from bonded sheets by laser singulation followed by end termination. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:30 AM

(EMA-S1-043-2017) Energy Harvesting from Vehicles Using a Pavement Embedded Piezoelectric Generator

G. Yesner^{*1}; A. Safari¹; 1. Rutgers University, USA

Non-resonant sources of mechanical energy, such as the stress induced in pavement from the loading of a vehicle, can be harvested using a novel piezoelectric transducer. The challenge of capturing the energy from this type of loading is matching the elastic modulus of the piezoelectric transducer to that of the road surface in order to facilitate efficient transfer of stress into the piezoelectric. Ceramic or multilayer transducers are too stiff and macro fiber composites are too flexible for efficient energy transfer. Transducers such as the cymbal have medium stiffness and can be further fine-tuned to match the stiffness road surface by changing the end cap material and geometry. A novel transducer designed utilizing a uniquely electroded and poled square ceramic along the length. The new transducer, called bridge due to its shape, greatly enhances the effective d_{33} coefficient at least two times (19,000 pC/N) compared to the conventional poled transducer. Transducers of the new design were fabricated and used to prototype a piezoelectric generator. A module containing 64 transducers was assembled and loaded with a force comparative to a small vehicle and repeated to simulate traffic. The output power of the energy harvesting device was used to power LEDs. The piezoelectric generator embedded in the pavement of a road would be an excellent source of power for off-grid sensors and electronics.

11:45 AM

(EMA-S1-044-2017) $\text{Bi}(\text{Zn}_{0.5}\text{Ti}_{0.5})\text{O}_3$ - BaTiO_3 Dielectric Composites Produced via Freeze-Casting

E. Gorzkowski^{*3}; E. Patterson³; M. A. Beuerlein²; G. L. Brenneka¹; 1. Colorado School of Mines, USA; 2. Colorado School of Mines, USA; 3. US Naval Research Lab, USA

In previous research freeze-casting was used to construct ceramic-polymer composites in which the two phases are arranged in an electrically parallel configuration. By doing so, the composites exhibit dielectric constant (K) up to two orders of magnitude higher than that of composites with ceramic particles randomly dispersed in a polymer matrix. This technique has been successful with both an aqueous and camphene based ceramic slurry that is frozen uni-directionally to form templates such that ceramic aggregates are aligned in the temperature gradient direction. Freeze-casting is a versatile processing technique that has been demonstrated to work with many ceramic systems. In this paper we will discuss the continued study of freeze-cast processing of composites based around non-saturating $\text{Bi}(\text{Zn}_{0.5}\text{Ti}_{0.5})\text{O}_3$ - BaTiO_3 ceramics for use in high power capacitor applications. The processing parameters (mold material, particle size, etc.), composite dielectric properties, and composite microstructure will also be presented.

12:00 PM

(EMA-S1-045-2017) Surface modification of flexible, ultra-thin glass based dielectrics to enhance capacitance

A. Mahadevegowda^{*1}; C. Johnston¹; P. S. Grant¹; 1. University of Oxford, United Kingdom

The purpose of this work was to devise and test a scalable processing technique to enhance the capacitance of glass-based capacitors by modifying the glass surface at a nanoscale. The systematic effect of this modification on the dielectric properties was studied and correlated to the observed nanostructure. Flexible capacitors based on ultra-thin glass (30 μm thick) were self-masked via a scalable vacuum based deposition technique and then preferentially etched to produce a controlled topography. Surface analysis was carried out before and after the treatment using atomic force microscopy (AFM) and scanning electron microscopy (SEM). The self-masked and etched samples showed higher capacitance than the as-received samples. AFM studies revealed the presence of nanoscale peaks

(~25 nm high), which were well-distributed across the glass surface. SEM studies showed that the masking material depleted with etching time. The percentage depletion of masking material and the roughness measurements revealed the cause of the formation of high surface area features, and were correlated to the observed enhancement in the capacitance, which was in-line with predictions and met the research objective. We believe that our novel approach improves the prospects of ultra-thin glass as a promising dielectric, which can be processed on a large scale, for example in a roll-to-roll fashion.

Lead Free Piezoelectrics I

Room: Coral B

Session Chair: Ke Wang, Tsinghua University

8:30 AM

(EMA-S1-046-2017) Peculiarities in the structure and dielectric properties of $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - BaTiO_3 (Invited)

R. Ranjan^{*1}; B. Rao¹; D. Khatua¹; I. Indian Institute of Science, India

The $(1-x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $(x)\text{BaTiO}_3$ piezoceramic shows enhanced piezoelectric properties at $x = 0.06$. While x-ray powder diffraction pattern suggests a cubic structure of $x = 0.06$, neutron powder diffraction reveals weak superlattice reflections which cannot be explained based on the conventional description of the P4bm + R3c phase coexistence model. Our study suggests a long period modulated structure in the unpoled state of $x = 0.06$. This composition shows maximum dielectric dispersion. We show that the precursor effect leading to the cubic-like structure sets in at $x = 0.03$, when structural state of the system changes from Cc + R3c for $x < 0.03$ to R3c + "cubic" for $0.03 \leq x < 0.06$. The long period structural modulation persists even in the tetragonal phase region up to $x = 0.20$. The crossover from a modulated tetragonal phase to a non-modulated tetragonal phase also coincides with the system exhibiting maximum tetragonality at this composition. Our study suggests that $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - BaTiO_3 system is structurally very complex in nature, and that long-period modulation plays crucial role in influencing its dielectric, ferroelectric and piezoelectric properties.

9:00 AM

(EMA-S1-047-2017) Recent Developments on Lead Free Ferroelectric Materials

S. Zhang^{*1}; Y. Qin²; J. Zhang²; 1. University of Wollongong, Australia; 2. Shandong University, China

Lead-Free piezoelectric ceramics have been actively investigated over the past 10 years because of potential environmental regulations. KNN-based and BNT-based ceramics with the perovskite structure are potential candidates for PZT replacement. The domain structure is a critical factor determining the dielectric and piezoelectric properties of ferroelectric materials. In this abstract, the domain structures of several KNN-based and BNT-based ceramics with different crystal phases and dopant, have been investigated. Short domain segments (before poling) and long domain stripes (after poling) were found to be typical domain configurations for KNN-BNKKZ. The reduced elastic energy, lattice distortion, and internal stress, due to the coexistence of R and T phases, result in much easier domain reorientation and domain wall motion, responsible for the high piezoelectric properties, being on the order of 460 pC/N, in which the extrinsic contribution from irreversible domain switching was estimated to be around 50% of the total piezoelectricity. Minor piezoelectric property variations (<6% over a temperature range from -50 to 100°C) were observed as a function of temperature, showing a good thermal stability. In addition, nanodomains (50 ± 2 nm) were found to be assembled into domain stripes after poling, believed to benefit the high piezoelectric properties but not causing much thermal instability due to the small quantity.

9:15 AM

(EMA-S1-048-2017) Structural and Piezoelectric Properties of CuO-added $0.96(\text{Na}_{0.5}\text{K}_{0.5})(\text{Nb}_{1-x}\text{Sb}_x)\text{O}_3$ - 0.04SrZrO_3 Lead-free Piezoelectric Ceramics

K. Lee^{*1}; D. Kim¹; J. Park¹; S. Cho¹; S. Nahm¹; 1. Korea University, Republic of Korea

The CuO-added $0.96(\text{Na}_{0.5}\text{K}_{0.5})(\text{Nb}_{1-x}\text{Sb}_x)\text{O}_3$ - 0.04SrZrO_3 ceramics with $x = 0 \sim 0.06$ have been sintered at low temperature of 1000°C. The CuO-related liquid phase was formed during the sintering process and assisted the densification of the specimens. All the specimens have a high relative density ($\geq 95\%$ of the theoretical density). Crystal structure of the specimen with $x = 0.0$ is orthorhombic and the orthorhombic and tetragonal transition temperature decreased with the increase of Sb_2O_5 . On the other hand, rhombohedral and orthorhombic transition temperature was near 10°C and it did not change with the addition of Sb_2O_5 . For the specimen with $x = 0.055$, the structure consisting of orthorhombic and tetragonal structures is considered to be formed. The detailed crystal structure of this specimen was identified using the Rietveld analysis. Grain size of the specimen increased with the increase of Sb content and the specimen with $x = 0.055$ has the average grain size of approximately 5.0 μm . The d_{33} , $\epsilon^T_{33}/\epsilon_0$ and k_p values of the specimen increased with the increase of x and the maximum d_{33} of 318 pC/N, $\epsilon^T_{33}/\epsilon_0$ of 1700 and k_p of 0.41 were obtained from the specimen with $x = 0.055$. The increases of piezoelectric properties were explained in term of the variations of crystal structure and grain size.

Lead Free Piezoelectrics II

Room: Coral B

Session Chairs: Steven Milne, University of Leeds; Rintaro Aoyagi, National Institute of Advanced Industrial Science and Technology

10:00 AM

(EMA-S1-049-2017) Domain Relaxation Behavior in CaZrO_3 Doped (K, Na) NbO_3 -based Ceramics (Invited)

K. Wang^{*1}; J. Li¹; 1. Tsinghua University, China

The development of lead-free piezoceramics has attracted great interest because of growing environmental concerns. Recently a promising composition of CaZrO_3 modified (K,Na) NbO_3 (KNN) materials has been developed, which demonstrates a large piezoelectric coefficient d_{33} above 350 pC/N at room temperature. Most intriguingly, the ceramic shows excellent temperature-insensitive strain behavior as well as high resistance towards electrical cycling conditions, which is very suitable for actuator applications. In this study, we demonstrate that ferroelectric domain relaxation is crucial for obtaining large piezoelectric strain in CaZrO_3 modified KNN materials. It is observed that a very high unipolar strain (0.21 % at 6 kV/mm) could be obtained in CaZrO_3 modified KNN ceramics by spark plasma sintering (SPS) method. Compared with the same material by normal sintering (NS), the SPSed samples are featured with enhanced large signal d_{33}^* from 340 pm/V to 415 pm/V at 4 kV/mm, and decreased small signal d_{33} from above 300 pC/N to 185~195 pC/N. The contrast effects of SPS processing on d_{33}^* and d_{33} are investigated by checking phase structure, ferroelectric and piezoelectric properties, with special consideration of CaZrO_3 doping level. Besides, local domain structures are studied by piezoresponse force microscopy (PFM). The results indicate that domain stability may be responsible for the gap between d_{33}^* and d_{33} .

10:30 AM

(EMA-S1-050-2017) Performance of Lead-free Dielectric and Piezoelectric Ceramics over Extended Temperature Ranges (Invited)

A. Zeb¹; D. Hall²; S. Jan¹; J. Li³; G. Wang⁴; F. Zhu⁵; S. J. Milne^{2*}; 1. Islamia College, Pakistan; 2. University of Leeds, United Kingdom; 3. Tsinghua University, China; 4. Manchester University, United Kingdom; 5. Shanghai Synchrotron Radiation Facility, China

Developing lead-free electroceramics with high relative permittivity or high electromechanical strains over wide temperature ranges presents a number of challenges. Here we report the properties and potential operating temperatures of dielectric and piezoelectric materials based on relaxor ferroelectrics derived from BaTiO₃ or M_{0.5}Bi_{0.5}TiO₃ (M = Na, K). Composition-structure-property relationships will be discussed for dielectrics with stable relative permittivity and low dielectric loss tangent over the technologically important -55°C to 300°C temperature range, and for a novel piezoelectric ceramic with depolarisation temperatures of ~220°C. The potential relevance of the materials for device applications will be considered.

11:00 AM

(EMA-S1-051-2017) Additive Effects on Electrical Properties of (Na,Ba)(Nb,Ti)O₃ Lead-free Piezoelectric Ceramics (Invited)

R. Aoyagi^{*1}; 1. National Institute of Advanced Industrial Science and Technology, Japan

Sodium niobate NaNbO₃ is well known antiferroelectric materials and its solid solutions between other perovskites shows ferroelectricity. The author (R.A) has studied electrical properties of solid solution (1-x)NaNbO₃-xBaTiO₃ (NNBTx) system as lead-free piezoelectric ceramics. NNBTx shows good piezoelectric constant d₃₃ of ~150 pC/N at x=0.10. However, their higher sintering temperature for preparing the high dense sample becomes a problem for NNBTx because of Na is easily volatilized during at high temperature. In this study, to lower sintering temperature and to improve electrical properties, the additive effects of NNBTx were investigated. Oxide and fluoride of MnCO₃, CuO, MO, LiF, and NaF were chosen as additives for sintering aid and/or harden elements. It was found that LiF was effective sintering aid in NNBTx. Almost same piezoelectric properties were obtained for LiF-added NNBTx although 200°C lower sintering temperature. Mn is known as harden element of perovskite piezoelectric ceramics but Mn-added NNBTx ceramics did not show hard piezoelectric properties. The phase transition temperature T_{OT} is remarkably decreased by Mn addition. That of NNBT0.06 decreased 130°C to near room temperature. As a result, piezoelectric constant d₃₃ and coupling factor were increased and mechanical quality factor was decreased.

11:30 AM

(EMA-S1-052-2017) Ferroelectric, piezoelectric, and structural studies of novel Bi-based perovskites

M. Dolgos^{*1}; 1. Oregon State University, USA

Due to the environmental impact of lead, there is a considerable focus on the synthesis of lead-free piezoelectric materials. Pb(Zr,Ti)O₃ (PZT) is the current industry standard for piezoelectric ceramics, but has a major disadvantage in that it contains lead, which is increasingly regulated. Our understanding of the high piezoelectric response in PZT is a direct result of the incredibly detailed structural studies that have been performed. Unfortunately, the same level of detail has not been applied to the lead-free counterparts of PZT. While some structural studies have examined both the average structure and local distortions of important lead-free piezoelectrics, there is currently not enough information to form a hypothesis about why PZT outperforms the lead-free alternatives. This talk uses a few examples to highlight the importance of obtaining a comprehensive structural description of lead-free piezoelectric materials in order to understand their properties and make new materials via rational design.

11:45 AM

(EMA-S1-064-2017) Formation and Microstructure of KNbO₃ Platelets Synthesized using K₄Nb₆O₁₇·nH₂O Precursor

Y. Ko^{*1}; H. Xu²; S. Nahm¹; 1. KU-KIST Graduate School of Converging Science and Technology, Republic of Korea; 2. Korea University, Republic of Korea

The KNbO₃ (KN) platelets were synthesized by annealing the K₄Nb₆O₁₇·nH₂O (KNOH) precursor at 700°C for 6 h for the first time. In general, the KNOH precursor has been solvothermally formed from the K_{8-x}H_xNb₆O₁₉·nH₂O intermediate phase which can be hydrothermally synthesized using KOH and Nb₂O₅ raw materials. However, in this work, the KNOH precursor was solvothermally produced from the KOH and Nb₂O₅ raw materials. In order to synthesize the homogeneous KN platelets, various amount of the K₂CO₃ was added during the annealing of KNOH. When the amount of K₂CO₃ is less than 20 wt%, the KNOH precursor was remained and the octahedral KN phase was formed when the amount of K₂CO₃ exceeded 30 wt%. The homogeneous orthorhombic KN platelets were well formed with 20 ~ 30 wt % of the K₂CO₃. The average size of KN plates was approximately 4~ 5 μm with a thickness of 0.3 μm. The growth direction of these KN platelets is [001]. The detailed synthesize processes and the formation mechanism of the KN platelets will be discussed in this work.

12:00 PM

(EMA-S1-054-2017) Depolarisation of Na_{0.5}Bi_{0.5}TiO₃-based Relaxors and the Resultant Double Hysteresis Loops

S. Huband^{*1}; P. A. Thomas¹; 1. University of Warwick, United Kingdom

The temperature induced depolarisation of (1-x-y)NBT - xBT - yKNN ceramics has been investigated using polarisation - electric field loops, current density - electric field loops, dielectric measurements, thermally stimulated depolarisation current measurements and x-ray diffraction. T_d values were calculated using the thermally stimulated depolarisation current measured in each furnace to allow comparison of results between techniques. T_d closely agreed with the values determined from the dielectric anomalies commonly referred to as T_{F-R} in the literature. T_d determined using pinching of polarisation - electric field loops was 2-9 K higher and was shown not to be from an antiferroelectric structure; pinching occurs as the induced ferroelectric phase becomes unstable and returns to its unpoled relaxor state. The ergodic and non-ergodic behaviour of relaxors and their relationship to antiferroelectrics are discussed.

12:15 PM

(EMA-S1-055-2017) Synergistically Enhanced Piezoelectricity and Temperature Stability in Potassium-Sodium Niobate Lead-free Ceramics

T. Zheng^{*1}; J. Wu¹; 1. Sichuan University, China

It has proven difficult to simultaneously achieve high piezoelectric performance and good temperature stability in KNN-based systems. Moreover the physical origin for its high piezoelectricity is still unclear, which makes property optimization without resort. Here we report the successful achievement of a giant piezoelectric coefficient (d₃₃) of 525 pC/N in KNN-based ceramics with high temperature stability (less than 10% variation for electric field-induced strain from 27°C to 80°C) through manipulating the rhombohedral-tetragonal (R-T) phase boundary. The structural origin of the high piezoelectric performance can be attributed to its hierarchical nano-domain architecture. The local structure inside nanodomains is the coexistence of R and T nanotwins. Derived from such nanoscaled structural coexistence, the physical origin of high piezoelectric performance can be attributed to low domain wall energy and nearly vanishing polarization anisotropy, which facilitates easily polarization rotation between different states and leads to high properties. We believe that the new breakthrough will open one window for the practical applications of KNN-based ceramics.

S3: Ceramic Photonic Materials and Applications

Ceramic Photonic Materials and Applications I

Room: Mediterranean C

Session Chairs: Juejun Hu, Massachusetts Institute of Technology;
Yiquan Wu, Alfred University

8:30 AM

(EMA-S3-001-2017) Hexagonal boron nitride epilayers: Growth, optical properties and device applications (Invited)

J. Lin^{*1}; H. Jiang¹; I. Texas Tech University, USA

Hexagonal boron nitride (h-BN) possesses extraordinary physical properties including wide bandgap ($E_g \sim 6.5$ eV), high temperature stability and corrosion resistance, and large optical absorption and thermal neutron capture cross section. In this talk, a brief overview of synthesizing wafer-scale h-BN epilayers by MOCVD will be presented. It was shown that the unique 2D structure of h-BN induces exceptionally high density of states and large exciton binding energy of about 0.7 eV, which results in high optical absorption and emission intensity. The most dominant impurities and deep level defects in h-BN epilayers were identified to be related to nitrogen vacancies. P-type conduction and diode behaviors in the p-n structures consisting of p-hBN/n-AlGaIn have been demonstrated. As deep UV photodetectors, h-BN detectors exhibit a peak responsivity at 217 nm with virtually no responses for below bandgap excitation. Neutron detectors incorporating a 43 μm thick B-10 enriched h-BN epilayer deliver a detection efficiency of 51.4% for thermal neutrons, which is the highest reported for semiconductor-based neutron detectors. It is our belief that h-BN will lead to many potential applications from deep UV emitters and detectors, radiation detectors, to novel 2D photonic and electronic devices.

9:00 AM

(EMA-S3-002-2017) Flexible photonics: Photonic integration with a new twist (Invited)

J. Hu^{*1}; I. Massachusetts Institute of Technology, USA

Glass and ceramic materials are often brittle and therefore usually cannot sustain large deformation. In this talk, we will challenge this conventional wisdom and examine novel mechanical and optical design strategies to impart extraordinary mechanical flexibility to photonic devices made out of fragile glasses and glass ceramics. Our rational design approach has led to passive integrated photonics devices capable of sustaining heavy-duty bending down to sub-millimeter radius or repeated stretching deformation with > 40% tensile strain. We will also report the demonstration of active optoelectronic component integration on flexible substrate platforms.

9:30 AM

(EMA-S3-003-2017) Quantized Charging and Property-Control of Single-Photon Emission from Site-Controlled III-Nitride Quantum Dots (Invited)

H. Deng^{*1}; I. University of Michigan, USA

Semiconductor quantum dots (QDs) provide an on-chip platform to generate single photons and isolate single charges for diverse applications to quantum information science. Most work has focused on self-assembled III-As QDs, which are limited in their operating temperature and integration. Here we demonstrate scalable III-N QDs with precisely controlled positions and dimensions. We measure single photon above liquid nitrogen temperature. We show control of the wavelength and polarization of the emission by size and shape of the QDs. We furthermore demonstrate quantized charging in the QDs, which paves the way for coherence spectroscopy and quantum information processing with III-N. The InGaIn QDs we use are lithographically defined at chosen positions and lateral sizes within a few nanometer precision. They feature

sub-nanometer linewidth, nano-second decay and single photon emission at higher temperatures than self-assembled ones. They share similar structures as nitride-based LEDs, readily integrated with electrical control capabilities. Single photon emission was confirmed via anti-bunching. Quantized charging was measured via the corresponding excitonic emission, showing sudden changes in the resonances and dipole moments, and disappearance of the fine-structure splitting. Electro-luminescence was observed at bias voltages above 2V.

10:30 AM

(EMA-S3-004-2017) Spatially Oriented Plasmonic 'Nanogratings' (Invited)

W. Li^{*1}; C. Gu¹; A. Cui¹; Z. Liu¹; I. The Institute of Physics, China

Metamaterials (MMs) have stimulated enormous research efforts in recent years. Fascinating optical properties, such as negative index, super-resolution and electromagnetic invisibility, have been explored in three-dimensional (3D) MMs. The key motivation in producing 3D MMs has always been the realization of structures with effective constituent properties that can be tuned in all propagation directions at various frequencies. However, up to now, to scale down 3D MMs for applications at higher frequencies, for example in the visible regimes, is still a challenge. Here, we review and report the application of FIB nano-patterning of thin film structures followed by ion-beam irradiation induced in-situ folding for the direct fabrication of substrate-free 3D plasmonic nanostructures and the observation of their unusual optical and sensing characteristics. Structure with unusual Fano resonances with a sensitivity of 2,040 nm per refractive index unit in the near infrared region were obtained. Meanwhile, Au nano units of different shapes with specifically designated orientations, were fabricated. Experimental measurements and simulation results show that such structures offer an additional degree of freedom for adjusting optical properties with the angle of inclination, in addition to the size of the structures. This may open up prospects for the fabrication of 3D nanostructures as optical interconnects, focusing elements and so on.

11:00 AM

(EMA-S3-005-2017) Electrically conductive glass-carbon composites (Invited)

G. Tao^{*1}; S. Chen¹; S. J. Pandey¹; A. Abouraddy¹; R. Gaume¹; I. University of Central Florida, USA

In this talk, we report the synthesis and characterization of a glass-carbon composite with high electrical conductivity in excess of 1800 S/m at the room temperature.

11:30 AM

(EMA-S3-006-2017) Comparative Study on Field Assisted Sintering and Hot Pressing of ZnS-CaLa₂S₄ Infrared Optical Ceramics (Invited)

Y. Li^{*1}; Y. Wu¹; I. Alfred University, USA

Compared with conventional hot pressing, the Field Assisted Sintering Technique (FAST) is an innovative way to consolidate ceramics in a manner which produces limited grain growth at reduced temperatures. In the present work, two pressure-assisted sintering routes, FAST and hot pressing, were applied to consolidate ZnS-CaLa₂S₄ composite infrared optical ceramics for application in harsh environments. A ZnS-CaLa₂S₄ composite powder was first produced by high-energy ball milling of ZnS nanopowder, synthesized by a wet chemical route, with commercial CaLa₂S₄ powder. Microstructural analysis was performed to correlate the microstructure and morphology of the composite ceramics with different ball milling and sintering parameters. Comparison of the phase composition and microstructural features of the ZnS-CaLa₂S₄ ceramics was performed to investigate the grain growth and sintering mechanisms of the two sintering techniques. Optical, mechanical and electrical properties were further characterized and analyzed to better

understand the effect of sintering conditions, composite composition, and defect formation on the performance of the ZnS-CaLa₂S₄ composite ceramics.

12:00 PM

(EMA-S3-007-2017) Optical characterization of natural and synthetic diamonds and diamond nanoparticles (Invited)

H. Ye^{*1}; T. Ochalski²; 1. Aston University, United Kingdom; 2. Cork Institute of Technology, Ireland

Ideal diamond is a wide band-gap semiconductor with indirect energy gap of 5.45 eV at room temperature. Deep UV excitation assures excitation of not only ground electronic state but also all defect- and impurity-related bands and sub-bands present inside the band-gap. In an indirect gap crystal (Si or diamond) the radiative recombination of photo-excited electrons from conduction band to valence band by means of UV light emission is a process of extremely low probability. The most probable scenario in an optically-excited crystal is a cascade of phonon-related non-radiative recombination events, combined with an excitation of optically-active impurity or defects levels (usually visible phosphorescence). The most common impurity levels and bands in diamond are nitrogen donor (1.7 eV), boron acceptor (0.37 eV), phosphorous donor (0.6 eV), and Sulphur donor (0.39-0.52 eV). Steady-state photoluminescence can detect the presence of specific impurities or defect bands in the diamond crystals but is unable to quantify them. In this work time resolved photoluminescence (TRPL) of natural and CVD diamond crystals and diamond nano-particles will be studied in terms of quality comparison between artificial and natural stones. Additionally comparison between emission dynamics and Raman spectroscopy, typically used for assessing diamond quality, will be presented.

S4: Computational Design of Electronic Materials

Novel Phenomena at Interfaces and Heterostructures

Room: Coral A

Session Chair: Sungjong Woo, Korea Institute for Advanced Study

8:30 AM

(EMA-S4-017-2017) First-principles modeling of electronic states in perovskite oxide heterostructures (Invited)

S. Park¹; K. M. Rabe^{*1}; 1. Rutgers, the State University of New Jersey, USA

The electronic structure of bulk perovskite oxides can be dramatically modified by incorporation into short-period superlattices, two specific mechanisms being quantum confinement in the ultrathin layers and stabilization of nonbulk crystal structures, including polar structures. In this talk, I will describe the development of a first-principles approach, based on a Wannier function representation of electronic states, for predictive modeling of characteristic electronic states in thin layers and at interfaces, with examples including superlattices of BaSnO₃/LaSnO₃, SrCrO₃/SrTiO₃ and LaVO₃/SrVO₃. The potential for this method for solution of inverse problems, such as design of one-dimensional or transparent conductors, will be discussed.

9:00 AM

(EMA-S4-018-2017) First-Principles Design of Two-Dimensional Electron Gas in the Perovskite-Oxide-Based Interface Materials (Invited)

K. Yang^{*1}; 1. University of California, San Diego, USA

The perovskite-based oxide heterointerfaces between two wide-band-gap insulators are attracting increasing interests because of their novel electronic properties such as the two-dimensional electron gas (2DEG) at the interface that have potential applications in the next-generation nanoelectronic devices. In this talk, I will present

our recent work on the high-throughput design of the perovskite-based nonpolar/polar 2DEG systems based on polar catastrophe mechanism. Then I will show the possibility to produce 2DEG at the nonpolar/nonpolar and at the polar/polar perovskite heterointerfaces, separately, as well as their fundamental mechanisms. These research findings may provide some avenues to achieve 2DEG in the perovskite-oxide-based interface materials.

9:30 AM

(EMA-S4-019-2017) Carrier localization in transition-metal oxides (Invited)

A. Janotti^{*1}; 1. University of Delaware, USA

Transition-metal oxides form one of the most interesting class of solids, exhibiting a variety of structure and properties, such as ferroelectricity, magnetism, high dielectric constants, high ionic conductivity, and high-T_c superconductivity. In the subset that are semiconductors, such as TiO₂ and SrTiO₃, for example, the behavior of charge carriers and their interaction with phonons and point defects give rise to unusual properties that are observed in transport measurements and optical spectra. In particular, these materials are prone to the formation of small polarons, that can be trapped by defects and impurities. From the perspective of first-principles calculations, we will discuss the behavior of point defects, such as oxygen vacancies, the formation of small polarons, the interaction between them, and their effect on optical and charge transport properties in a series of transition-metal oxide semiconductors. Particularly, we will try and distinguish the properties of small polarons from the defects or impurities that originate them. The results will be used to interpret available experimental data.

10:15 AM

(EMA-S4-020-2017) Understanding the advantages of hexagonal WO₃ as an efficient photoanode for solar water splitting: A first-principles perspective (Invited)

T. Lee¹; Y. Lee¹; W. Jang¹; A. Soon^{*1}; 1. Yonsei University, Republic of Korea

Polycrystalline WO₃ has been suggested as an alternative photoanode material for the water splitting reaction.^{1,2} However, the band gap and band edge positions of the most commonly used γ -monoclinic WO₃ phase are found to be not optimal for effective water oxidation.³⁻⁵ In this work,⁶ by using first-principles density-functional theory calculations with an ab initio thermodynamic model, we demonstrate the potential advantage of using the hexagonal phase of WO₃ (h-WO₃ and its surfaces) over the larger band gap γ -WO₃ phase for the anode in water splitting. Notably, after addressing the relative thermodynamic stability of the various h-WO₃ surfaces, we carefully quantify and compare the electronic band structure of these two bulk phases of WO₃ (using their valence and conduction band edges as descriptors). We then provide a simple perspective as to illustrate how the surface band edges of h-WO₃ match up with the redox potential of water and other possible cathode materials.

10:45 AM

(EMA-S4-021-2017) Understanding the A-Cation Order Dependent Band Gap Variation in Ruddlesden-Popper Oxides

Y. Shin^{*1}; J. Rondinelli¹; 1. Northwestern University, USA

Here we examine the electronic structure of Ruddlesden-Popper (RP) oxides, focusing on (LaSr)AlO₄ and changes induced by cation order. This RP phase can be described as one perovskite block stacked along the [001] direction with an extra AO rock-salt layer interleaving the blocks. The partial connectivity allows further atomic scale control of Coulombic interactions within the structure, which enables design of novel electronic and optical properties. Recently the aluminate RP superlattice was predicted to show massive band gap variations, up to 200%, depending on the A cation ordering using first-principles electronic structure calculations. This variation was attributed to changes to the internal electrostatic potential and electric fields within the superlattice mediated by ionic

relaxations. We extend this concept, showing that longer period arrangements of the monoxide planes lead to greater control over the band gap and even its full collapse, i.e., metal-insulator transition is observed. Density functional theory calculations are used to investigate the underlying mechanism of this band gap variation. We conclude by summarizing our findings into a set of working principles for band gap control in layered oxides without changes in cation stoichiometry.

11:00 AM

(EMA-S4-022-2017) Phase-field modeling of magnetoelectric coupling in biferroic composite thin films with patterned interface

Y. Alvandi-Tabrizi^{*1}; W. Chan²; J. Schwartz²; 1. North Carolina State University, USA; 2. North Carolina State University, USA

The interfacial connectivity between the constituents plays a crucial role in the performance of the magnetoelectric (ME) biferroic composite films. Two successful approaches are multilayered thin films and nano-pillars embedded in a film; each has advantages and challenges. The strain coupling in a layered structure is impacted by the constraint imposed by the substrate, whereas, the vertical interfaces in films with nano-pillars span the entire thickness of the film, resulting in leakage problems. An ideal system for achieving high ME coupling through strain would be one containing vertical interfaces that are discontinuous in the field direction. A new design principle based on using patterned interface is proposed in this study. The patterning introduces three-dimensional interfaces consistent with the ideal geometry for ME coupling. A phase-field modeling technique implemented in COMSOL Multiphysics is employed to study the efficacy of such new design in improving the magnetoelectric coupling.

11:15 AM

(EMA-S4-023-2017) Electronic structure and band alignments of half-Heusler semiconductors for electronic applications

A. Sharan^{*1}; Z. Gui²; A. Janotti²; 1. University of Delaware, USA; 2. University of Delaware, USA

Half-Heuslers with 18 valence electrons are promising materials for electronics. However, data on basic properties, such as their electronic structure and band alignments are scarcely available. Here we explore two members of this large family of compounds, TiCoSb and TiNiSn, which can be grown on conventional III-V semiconductors and could potentially be integrated in III-V devices. We present results of first principles calculations of electronic structure and band alignments to conventional III-V semiconductors. Electronic structures are calculated using density functional theory within both the generalized gradient approximation and hybrid functional (HSE06). The results are discussed and compared to the available experimental data. This work was supported by US Department of Energy.

High-Throughput Approaches

Room: Coral A

Session Chair: Emmanouil Kioupakis, University of Michigan

11:30 AM

(EMA-S4-024-2017) Discovery of solar fuels photoanode materials by integrating high-throughput theory and experiment (Invited)

Q. Yan^{*1}; 1. Lawrence Berkeley National Lab, USA

High-throughput computing and materials databases, largely based on density functional theory (DFT), have recently enabled rapid screening of solid-state compounds with simulation for multiple properties and functionalities. These DFT-based databases and analytics tools have already been used to identify more than 20 new functional materials that were later confirmed by experiments across a number of applications. However, in photoelectrochemistry for

the renewable synthesis of solar fuels, efficient metal oxide photoanode materials – photoelectrocatalysts for the oxygen evolution reaction (OER) – remain critically missing. Forty years of experimental research has yielded just 12 metal-oxide photoanode compounds with band gap energy in the desirable 1.2 to 2.8 eV range that strongly overlaps with the solar spectrum. By integrating ab initio theory with experiments, we report the discovery of 12 vanadate oxide photoelectrocatalysts for water oxidation, doubling the number of known photoanodes in the target band gap range. Detailed analysis of these vanadate compounds confirms the role of VO₄ structural motifs and electronic band character in establishing an efficient photoanode, initiating a genome for photoanode materials and paving the way for a high-throughput-discovery and materials-by-design feedback loop that is broadly applicable for developing functional materials.

12:00 PM

(EMA-S4-025-2017) Functional Defects by Design: A High-Throughput Approach to Energy Materials Discovery

J. Balachandran²; L. Lin³; J. Ding¹; Y. Cheng³; J. Anchell³; R. Unocic³; N. Bassiri-Gharb¹; G. Veith³; W. Ren³; C. Bridges³; P. Ganesh^{*3}; 1. Georgia Institute of Technology, USA; 2. Oak Ridge National Lab, USA; 3. Oak Ridge National Lab, USA

Defects and impurities introduce localized heterogeneities in solids and decisively control the behavior of a wide range of energy technologies. Fuel cell materials, especially proton conducting fuel cells, are a quintessential example in this regard. Designing and developing solid oxide materials that can rapidly transport protons will enable us to develop the next generation proton conducting solid oxide fuel cells. We initially focus on the perovskite family of compounds (such as doped BaZrO₃). We benchmark our calculations against a wide range of experimental measurements such as Kelvin probe force microscopy (KPFM), inelastic neutron scattering (INS) and atom probe tomography (APT). To obtain better insights on why certain cubic perovskite/dopant combinations are better at conducting protons compared to others, we developed a high-throughput framework to perform ab initio calculations. We employ this approach to calculate proton transport properties in more than 120 cubic perovskite materials with different host atoms and dopants. The results obtained from these calculations enable us to obtain better insights on how material structure – such as atomic properties (electronegativity, ionic radius) and lattice properties (sub-lattice distortion) influences proton transport. We are training machine learning algorithms to this data to make new predictions.

12:15 PM

(EMA-S4-026-2017) Computational Prediction of Two-Dimensional Transition Metal Mono-Chalcogenides

B. Rijal^{*1}; J. T. Paul¹; M. Ashton¹; R. G. Hennig¹; 1. University of Florida, USA

Two-dimensional (2D) materials are a novel class of materials with different physical, electronic, and magnetic properties than their bulk counterparts and can have applications in sensing, catalysis, and energy storage. In this work, a single layer of copper telluride was chemically substituted with similar elements in the periodic table. We used the high-throughput MPInterfaces framework and density-functional theory to identify low-energy 2D materials and characterize their electronic and magnetic properties. Our calculations showed that the chemically substituted single layered transition metal mono-chalcogenides are most stable in the copper telluride structure. The formation energy of these compounds are low enough that they can be mechanically exfoliated or grown on substrates using CVD or MBE methods. We found metallic and magnetic properties in these materials that can have potential application as metallic contacts and transistors in semiconducting devices.

12:30 PM

(EMA-S4-027-2017) High-Throughput Data Generation and Screening of Transition Metal Dichalcogenides

L. Li^{*1}; I. Williamson¹; 1. Boise State University, USA

Transition metal dichalcogenides (TMDs) are of broadening research interest due to their electronic and energy applications. Having chemical formula MX_2 , where M is a transition metal and X is a chalcogen, there are many combinations to consider for materials-by-design exploration. Varying M elements and their polytypes yields different symmetric structures, enabling to optimize the electronic, optical and thermal properties of the materials to meet performance requirements. We screened more than 60 TMDs for their environmental impact, cost, structural stability, electrical, phonon, and thermal properties with a combination of first-principles approaches and Boltzmann transport theory. Our results identified the atomic weight, radius and oxidation state of transition metals as key factors to control the TMD material properties. This enables faster and more effective TMD selection and design. Doping and creating heterojunction in TMDs are two common processes to improve the properties, specifically for electronic and energy conversion devices. We screened the TMDs with 18 transition metal dopants and heterojunctions with different compositions and lattice mismatching in order to identify the structure-property relationships. In the presentation, we will discuss their effects and a set of TMD design and selection principles.

S8: Interfaces and Surfaces in Energy-Related Ceramic Materials

Interface Structures in Batteries

Room: Mediterranean A/B

Session Chair: Brian Sheldon, Brown University

8:30 AM

(EMA-S8-008-2017) Understanding the Surface of $LiMn_2O_4$ Spinel Cathodes with Aberration-Corrected HAADF STEM and EELS (Invited)

P. Ferreira^{*1}; 1. University of Texas at Austin, USA

As global energy consumption continues to rise, the importance of energy storage becomes very important. One of the most promising chemistries in lithium-ion batteries is $LiMn_2O_4$ (LMO), a spinel cathode which has both a high energy density and a high rate capability, but is plagued with cyclability problems. In the LMO system, cycling degradation is mainly due to the Mn disproportionation reaction ($2Mn^{3+} = Mn^{2+} + Mn^{4+}$) which creates soluble Mn^{2+} that is lost to solution. This loss from LMO leads to capacity degradation. In order to understand how LMO loses active material from its surface, it is crucial to determine the surface's atomic structure. In this paper, we use a combination of high-angle annular dark-field (HAADF) aberration-corrected scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) to identify the atomic surface structure and composition of LMO. We find, in as-processed LMO, a surface structure composed of Mn_3O_4 and a $Li_{1-x}Mn_2O_4$ subsurface layer due to surface reconstruction. These conclusions are based on Mn oxidation state and oxygen mapping with EELS as well as structural identification with HAADF STEM and STEM simulations. We also found the presence of Mn^{2+} at the surface and have identified oxygen loss as the mechanism by which the surface reconstruction occurs.

9:00 AM

(EMA-S8-009-2017) 2-D MnO_2 nanosheet assemblies: electrochemical intercalation at surface defect sites

S. Mixture^{*1}; P. Metz¹; P. Gao¹; 1. Alfred University, USA

Single and several-layer 2-D birnessite MnO_2 nanosheets were prepared via exfoliation of high-perfection starting microcrystalline powders and reassembled into 3-D porous structures. Controlled reduction of some of the tetravalent Mn led to tripling of the electrochemical charge storage capacity. X-ray total scattering was teamed with X-ray spectroscopy and related tools to probe both the meso-structure and the atomic defects of MnO_2 nanosheet assemblies, revealing a direct link between surface Mn defects and capacitance. We define a 'surface Frenkel' defect as critical in controlling the electrochemical charge storage, where the capacitance increased from about 150 F/g to over 350 F/g when by intentional reduction of some of the Mn to the trivalent state. In addition, the charge transfer resistance decreased from $\sim 18 \Omega$ to $\sim 3 \Omega$ and the cycling fade is improved markedly. X-ray PDF studies show unequivocally that the reduced Mn ions form surface Frenkel defects, wherein the Mn ions shift from locations in the planar nanosheet to the nanosheet surface, leaving a Mn vacancy in the sheet. Implications of the use of these characterization tools for study of related disordered 2-D solids and our resulting understanding of atomic scale defects in these 2-D entities will be considered.

In Situ Characterization of Interface Structure and Evolution (Joint session with Symposium 7)

Room: Mediterranean A/B

Session Chair: Paulo Ferreira, University of Texas at Austin

9:45 AM

(EMA-S8-010-2017) In situ characterization of battery materials by transmission x-ray microscopy (Invited)

J. Wang^{*1}; 1. Brookhaven National Laboratory, USA

Synchrotron based full field hard x-ray transmission x-ray microscopy (TXM) has emerged as a power tool to in situ or in operando non-destructively characterize microstructural evolution of electrode particles as the battery charging and discharging to correlate to the battery performance. The newly developed TXM at X8C beamline, National Synchrotron Light Source (NSLS) provides nano-tomography capability to track the microstructural evolutions in three dimensional (3D) at nanometer scale. It enables direct observation of morphological changes and chemical composition distributions in 3D within individual particles and throughout the electrode as cycling proceeds in an operating battery cell. Combined with x-ray absorption near-edge structure (XANES) spectroscopy, TXM-XANES provides in situ chemical mapping in 3D to track phase transformation in a battery to bring new shed into chemical reaction pathways. This talk will present unique features of the TXM and applications in battery materials.

10:15 AM

(EMA-S8-011-2017) Stress Evolution and Degradation Mechanisms at Interfaces in Energy-Related Ceramics (Invited)

B. W. Sheldon^{*1}; 1. Brown University, USA

The volume changes that are associated with composition variations in a solid can induce significant stresses, when these expansions or contractions are physically constrained. These phenomena are important in a variety of energy-related materials, where they lead to complex interactions between electrochemical and mechanical driving forces. We have employed in situ measurements of these stresses along with a variety of other in situ and ex situ characterization methods, to obtain critical information about how the relevant mechanisms operate in different types of materials. One example is ceria electrolytes in solid oxide fuel cells, where oxygen potential gradients across the electrolyte can lead to large stresses.

These stresses are significantly enhanced by grain boundary contributions that can be interpreted with space charge effects. In some Li ion battery cathodes, both oxygen non-stoichiometry and Li insertion and removal can lead to complex stress effects. Another area of interest in batteries is the solid-electrolyte interphase (SEI), where we have shown that stresses and SEI mechanical properties can be engineered to enhance the stability of these critical passivation layers.

10:45 AM

(EMA-S8-012-2017) Direct imaging of ion insertion and phase transition processes in WO_3 thin film electrodes

Y. Du^{*1}; Y. He²; S. Mao³; H. Xiao³; F. Gao⁴; L. Luo¹; C. Wang¹; 1. Pacific Northwest National Laboratory, USA; 2. University of Pittsburgh, USA; 3. University of Electronic Science and Technology of China, China; 4. University of Michigan, USA

Intercalation and conversion are two fundamental chemical processes for battery materials in response to ion insertion. The interplay between these two chemical processes has never been directly seen and understood at atomic scale. In this talk, I will present how we tune the structure and electronic properties of WO_3 epitaxial thin films, and use them as model electrode materials for in situ TEM studies. The atomic scale ion (Li^+ , Na^+ , and Ca^{2+}) intercalation and conversion reactions are revealed by STEM, EELS, NBD, and theoretical calculations. It is revealed that the initial reversible intercalation process leads to a monoclinic to cubic phase transition accompanied by an insulator to metal electronic transition. Upon further insertion, the foreign ion-oxygen bond formation destabilizes the transition-metal framework which gradually shrinks, distorts and finally collapses to an amorphous W and MxO ($\text{M}=\text{Li}$, Na , Ca) composite structure. I will also discuss how strained induced structural defects can significantly affect the ion transport processes. These studies provide an atomistic picture of the ion transport and reaction mechanisms, which are of essential importance for both secondary ion batteries and electrochromic devices.

S7: In situ Experiments of Microstructure Evolution and Properties

In Situ Experiments on Microstructural Evolution and Properties I (Joint session with Symposium 8)

Room: Mediterranean A/B

Session Chairs: Shen Dillon, University of Illinois at Urbana-Champaign; Wayne Kaplan, Technion - Israel Institute of Technology

11:00 AM

(EMA-S7-001-2017) Photovoltaic properties and microstructure in CdTe solar cells via Tomographic AFM (Invited)

J. Luria²; Y. Kutes²; K. Atamanuk²; A. Moore³; L. Zhang¹; E. Stach¹; B. D. Huey^{*2}; 1. Brookhaven National Laboratory, USA; 2. University of Connecticut, USA; 3. Colorado State University, USA

Computed Tomography (CT) with x-rays and TEM are increasingly employed for full 3-d analyses of microstructure and chemical composition. Investigations of properties, however, are limited to bulk measurements or surface studies typically with variations of AFM. With the advent of various sectioning methods, this is no longer a limitation. Accordingly, CT-AFM is introduced for 3-d property mapping. Specifically, investigations with polycrystalline thin film solar cells demonstrate the evolution of microstructure and properties through the 2 μm thickness of the CdTe absorbing layer. Contrast is based on layer-by-layer conductive-AFM mapping of the short circuit current or open circuit potential. The results clearly confirm extensive electron conductivity localized at grain boundaries. But CT-AFM also reveals a previously unexplored network of hole-conduction pathways along highly interconnected

planar defects. Grain to grain variations in local solar cell performance metrics, of more than 1 order of magnitude, are also mapped evidencing substantial heterogeneities for the photo-electric behavior of the inter- and intra- granular interfaces. In situ measurements such as CT-AFM, coupling properties and microstructure, may therefore be crucial to understanding and ultimately improving polycrystalline solar cells by optimizing the volume fraction of champion grains and interfaces.

11:30 AM

(EMA-S7-002-2017) Using in-situ electron microscopy methods to study the thermal degradation of nickel-based cathode materials (Invited)

E. Stach^{*1}; S. Hwang¹; K. Karki²; S. Kim³; W. Chang³; S. Whittingham²; G. Zhou²; 1. Brookhaven National Laboratory, USA; 2. Binghamton University, USA; 3. Korean Institute of Science and Technology, Republic of Korea

Intercalation-based $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ (NCA) and $\text{LiNi}_{0.3}\text{Co}_{0.3}\text{Mn}_{0.3}\text{O}_2$ (NCM) have been pursued as potential cathode materials for EV and HEV applications, because of their high energy density (~ 200 mAh/g) and lower cost. However, at elevated temperatures, the highly delithiated NCA/NCM electrodes release O_2 gas, preceded by the reduction of the transition metal (TM) ions and structural phase transitions (R-3m to Fd-3m to Fm-3m), which can cause catastrophic thermal runaway reactions with the electrolyte. Therefore, it is critical to understand the role that the release of O_2 plays in the migration of TM (Ni, Co, and Mn) cations during the various phase transition processes. In-situ and environmental transmission electron microscopy (ETEM) provide a unique platform where individual nanoparticles can be investigated for any morphological, structural or chemical changes, under external stimuli, in real-time. We use in-situ TEM to follow the course of these phase transitions as a function of temperature, and correlate them with electron energy loss spectroscopy (EELS) to track subtle chemical changes that occur near the surface region. In addition, we utilize ETM to understand the role oxygen plays in the rearrangement of the transition metal ions both at the surface and the bulk of the materials at elevated temperatures.

12:00 PM

(EMA-S7-003-2017) Imaging Dynamic Materials Processes in Liquids by (Scanning) Transmission Electron Microscopy (S/TEM) (Invited)

N. Browning^{*1}; 1. Pacific Northwest National Lab, USA

Many processes in materials science, chemistry and biology take place in a liquid environment – such as chemical conversions, the synthesis of nanoparticles, the operation of Li-ion or next generation batteries, and biological cellular functions. For these systems, the final desired outcome is a result of a series of complicated transients, where a change in the order, magnitude or location in each of the steps in the process can lead to a radically different result. Understanding and subsequently controlling the final outcome of the process therefore requires the ability to directly observe the transients as they happen. In this presentation, results demonstrating the use of in-situ liquid stages in aberration corrected (scanning) transmission electron microscopes (S/TEM) to quantify transient materials processes will be presented and the potential insights that can be gained by increasing the image acquisition speed and/or decreasing the electron dose will be described (dose fractionation and the controlled reduction of electron beam induced artifacts is the main challenge for in-situ microscopy). The benefits of compressive sensing and in-painting methods to acquire optimally sampled images and the use of pulsed photo-emission sources for sub-microsecond imaging in the Dynamic TEM (DTEM) will also be discussed.

S10: Interfacial Phenomena in Multifunctional Heterostructures: From Theory to Transport Processes

Synthesis and Characterization of Heterostructures and Superlattices

Room: Caribbean B

Session Chair: Dillon Fong, Argonne National Lab

8:30 AM

(EMA-S10-014-2017) Band Alignment at the $\text{SrZr}_{1-x}\text{Ti}_x\text{O}_3/\text{p-Ge}(001)$ Heterojunction and Surface Reactivity toward Water (Invited)

S. Chambers^{*1}; Y. Du¹; K. Stoerzinger¹; I. Pacific Northwest National Laboratory, USA

We are investigating the properties of high-quality epitaxial interfaces of $\text{SrZr}_{1-x}\text{Ti}_x\text{O}_3$ on p-Ge(001) prepared by molecular beam epitaxy. Our aim is to generate model electrode surfaces and interfaces for fundamental studies of the hydrogen evolution reaction associated with water splitting. We seek to determine the value of x at which the conduction band offset (CBO) is zero. Such a heterojunction would allow electrons photogenerated in the p-Ge to drift into the n-perovskite and then cross the interface into the aqueous solution to reduce H^+ , ideally without the need for a noble metal catalyst. Based on in situ, high-energy resolution x-ray photoelectron spectroscopy (XPS) measurements, our preliminary results indicate that a value of $x = 0.30$ reduces the CBO, which is 0.3(1) eV, to ~ 0.1 eV. Moreover, 0.4 eV of downward band bending has been detected in the p-Ge which further facilitates electron drift into the perovskite. In this talk, these and other results will be presented, including ambient pressure XPS measurements carried out at the Advanced Light Source to determine the extent of reaction of water with these surfaces.

9:00 AM

(EMA-S10-015-2017) Measuring Built-in Electric Fields in Oxide Heterostructures with X-rays (Invited)

R. Comes^{*1}; I. Auburn University, USA

Polar/non-polar interfaces in epitaxial oxide films have been a rich area of research for many years for emergent behavior. Recent work has branched out to explore ways to use these interfaces to engineer optical responses in materials as well. The interfacial dipole that results from the polar discontinuity at such interfaces can generate band bending and a built-in electric field near the interface, which may be used to separate optically-excited electron-hole pairs for enhanced photovoltaic and photocatalytic response. However, detailed characterization of the band structure is needed to understand both the origin of these phenomena and engineer their behavior. In this talk I will discuss our work using interfacial termination in polar/non-polar heterojunctions and superlattices to engineer electric fields in these materials. Using in situ x-ray photoelectron spectroscopy (XPS) characterization of the $\text{LaFeO}_3/\text{n-SrTiO}_3$ junction with differing interfacial termination, we extract the valence and conduction band alignment between the materials and show that we can tune the band alignment by interfacial engineering. In $\text{LaCrO}_3/\text{SrTiO}_3$ superlattices, we employ synchrotron standing wave XPS to examine the electronic dispersion of buried layers and show that by engineering alternating terminations between positively charged TiO_2 -LaO and negative CrO_2 -SrO interfaces a polarization is induced in each material.

9:30 AM

(EMA-S10-016-2017) Atomic Imaging Multifunctional Heterostructures and Heterointerfaces by Phasing Coherent Bragg Rods (Invited)

H. Zhou^{*1}; I. Argonne National Lab, USA

A subtle modification near an interface can have a decisive effect on properties of the collective as well as each individual. A compelling case manifesting such subtlety is oxide heterostructures and heterointerfaces exhibiting fascinating emergent behaviours due to numerous combinative contributions of atomic structures and chemistries. Surface/interface X-ray scattering from modern synchrotron sources integrated with phase retrieval direct methods provides a very powerful toolkit to decipher the interfacial subtlety. In this talk, I will firstly give a brief introduction of how to obtain atomic mapping of oxide heterostructure and heterointerfaces with sub-Ångström resolution by phase retrieving coherent Bragg rods. In the following, I will demonstrate a few recent studies in the exploration of oxide heterostructures and heterointerfaces for information and energy applications by applying the direct method, such as revealing structural motifs responsible for various quantum states, catching structural perturbations in response to internal and external electric fields, and differentiating at the atomic-layer level the complicated cation distribution. In the end, I will give a short commentary on future opportunities in X-ray studies of oxide interfaces and heterostructures enabled by the exciting advancements towards ultimate storage rings.

10:30 AM

(EMA-S10-017-2017) Synthesis of polar oxide superlattices from centrosymmetric constituent layers (Invited)

S. May^{*1}; I. Drexel University, USA

There has been rapid growth of interest in designing layering-induced polar crystal structures in transition metal oxide superlattices as a means to realize new combinations of functionality in these materials. In this talk, I will present experimental efforts to realize these heterostructures using oxide molecular beam epitaxy. In ABO_3 perovskite based structures, the influence of strain and substrate imprinting on the orientation of the octahedral rotation pattern ($a^-a^+c^-$ vs $a^-a^+c^+$) will be discussed. It will be shown that growth on (001)-oriented orthorhombic substrates provides the most deterministic route to realizing the necessary $a^-a^+c^+$ pattern for polar superlattices. The structure and properties of $(\text{LaFeO}_3)_n/(\text{EuFeO}_3)_n$ superlattices grown on these substrates will be presented. Finally, brownmillerite $(\text{CaFeO}_{2.5})_n/(\text{SrFeO}_{2.5})_n$ superlattices will be shown to be non-centrosymmetric; the polar behavior in these crystals arises from ordering of both A-site cations and oxygen vacancies as predicted by density functional theory. The work was performed in collaboration with Amber Choquette and Eun Ju Moon (Drexel University); Joshua Young and James Rondinelli (Northwestern University); Debangshu Mukherjee, Greg Stone, Venkat Gopalan, and Nasim Alem (Penn State University). S.J.M. was supported by the National Science Foundation under grant number DMR-1151649.

11:00 AM

(EMA-S10-018-2017) The Influence of Surface Atomic Structure on Solid State Electrochemistry (Invited)

M. Riva^{*2}; M. Kubicek⁴; X. Hao⁴; S. Gerhold²; G. Franceschi²; M. Schmid²; H. Hutter³; J. Fleig³; C. Franchini⁵; B. Yildiz³; U. Diebold²; 1. Massachusetts Institute of Technology, USA; 2. TU Wien, Austria; 3. TU Wien, Austria; 4. Yanshan University, China; 5. University of Vienna, Austria

Perovskites are widely used materials for enabling oxygen reduction and evolution reactions, which limit the efficiency of energy conversion technologies. In solid-state electrochemistry, the reactivity on perovskites is interpreted in terms of the availability of oxygen vacancies, or the ease of electron transfer. None of these standard reactivity models consider the role of the atomic structure

of surfaces. In the present contribution I will show that the surface atomic structure plays a crucial role in affecting oxygen exchange on $\text{SrTiO}_3(110)$, which we can reproducibly, and reversibly prepare with several surface phases, all of which are based on families with $(n \times 1)$, and $(2 \times m)$ symmetries, with their surfaces composed of tetrahedrally-, and octahedrally-coordinated Ti atoms. Using a host of surface science techniques (STM, LEED, XPS,...) we find that these structures are remarkably stable under realistic conditions for oxygen-exchange reactions. We used two different ion-based spectroscopy techniques to quantify the ^{18}O exchange and found that the reactivity of these two reconstructions differs by a factor of three. From DFT calculations and electron spectroscopic measurements we rule out that this difference is due to oxygen vacancies or to differences in electronic structure. Instead the structural details determine the interaction with molecular oxygen. Work supported by FWF (FOXS) and ERC (A.G. 'OxideSurfaces').

11:30 AM

(EMA-S10-019-2017) Exploring low dimensional electron system at transition metal oxides: Create and Control (Invited)

M. Radovic^{*1}; I. Paul Scherrer Institut, Switzerland

Transition Metal Oxides (TMOs) exhibit unique and multifunctional electronic properties (such as high-temperature superconductivity, colossal magnetoresistance, metal-insulator transitions, etc.) directly related to the spin and orbital degrees of freedom of the transition metal d-states. Furthermore, their iso-structural nature permits realization of heterostructures where novel unexpected electronic properties take place. This is the case of oxide-2DEGs, which recently showed extraordinary occurrences, including interfacial magnetism, large tuneable spin-orbit coupling and indications of topological states. In my talk, I will present spin resolved Angle Resolved Photoemission Spectroscopy (ARPES) studies of the low dimensional electron gas at SrTiO_3 [1, 2, 3], TiO_2 -anatase and BaTiO_3 showing that these materials have capability for the realization of TMO based spintronic device.

12:00 PM

(EMA-S10-020-2017) Interfaces in a $\text{VO}_2(\text{B})/\text{SrTiO}_3$ heterostructure

X. Gao^{*1}; S. Lee¹; M. F. Chisholm¹; H. Lee¹; I. Oak Ridge National Laboratory, USA

Fundamental understanding of interfaces of thin film electrodes is important to develop energy storage and generation devices. Among electrode candidates, the bronze phase $\text{VO}_2(\text{B})$ has attracted attention due to its unique open structure ideal for ion conduction. We have established the epitaxial growth technique for $\text{VO}_2(\text{B})$ on SrTiO_3 . Such heterostructures provide an intriguing interface, where two materials with a large crystallographic symmetry meet, i.e., the low symmetry $\text{VO}_2(\text{B})$ on the high symmetry SrTiO_3 . In this work, direct observations using state-of-the-art scanning transmission electron microscopy (STEM) unveil an intriguing interfacial layer that enables epitaxial growth of strain-free, monoclinic $\text{VO}_2(\text{B})$ thin films on perovskite SrTiO_3 . We have observed an ultrathin (2-3 unit cells) interlayer best described as highly strained $\text{VO}_2(\text{B})$ nanodomains combined with an extra $(\text{Ti,V})\text{O}_2$ layer on the TiO_2 terminated STO (001) surface. By forming a fully coherent interface with the STO substrate and a semi-coherent interface with the strain-free epitaxial $\text{VO}_2(\text{B})$ film above, the interfacial bi-layer enables the epitaxial connection of the two materials despite their large symmetry and lattice mismatch. *This work was supported by the U.S. Department of Energy, Office of science, Basic Energy Sciences, Materials Sciences and Engineering Division.

12:15 PM

(EMA-S10-021-2017) Dislocation-free strain relaxation in $\text{RuO}_2(110)$ epitaxial films

Y. Wang^{*1}; A. Wong²; A. Herklotz¹; T. Z. Ward¹; H. Weitering²; P. Snijders¹; 1. Oak Ridge National Lab, USA; 2. The University of Tennessee, USA

Heteroepitaxy is usually accompanied by lattice mismatch and strain. Above a critical thickness, this strain is relieved by dislocations or 3D growth and negatively affects the electron mobility of heteroepitaxial layers in electronic devices. Here, we report a strain relief mechanism on atomically flat $\text{RuO}_2(110)$ thin films as a complementary to the formation of dislocations. Atomically flat $\text{RuO}_2(110)$ single crystal films were prepared on $\text{TiO}_2(110)$ substrates via Molecule Beam Epitaxy. A low density of stacking faults due to dislocations is observed in STM on films that are thicker than ~ 18 monolayers (ML). The density of dislocations increases with the film thickness and saturates at ~ 27 ML. With decreasing temperature below 300 K, an increasing density of ridge-shaped structures appears on the terraces for films thicker than ~ 4 ML. The corrugation of these ridges is around 60 pm, i.e. significantly less than the step height (3.2 Å). Their density is also thickness dependent: at 100 K the ridge density peaks at 8 ML and then decays to almost zero at 33 ML, anticorrelating with the dislocation concentration as a function of thickness. Furthermore, the ridges on thin $\text{RuO}_2(110)$ films significantly affect the temperature dependent electrical resistance. Our observation suggests there is a new strain relief mechanism that does not involve bond breaking, and that this competes with dislocation-mediated strain relief.

S11: Ion Conducting Ceramics

Ion Conduction for Energy Storage

Room: Caribbean C

Session Chair: Claire Xiong, Boise State University

8:30 AM

(EMA-S11-001-2017) Synthesis of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Garnet Nanowires and Evaluation as Ceramic Fillers in Composite Polymer Electrolytes (Invited)

T. Yang¹; C. K. Chan^{*1}; 1. Arizona State University, USA

Lithium lanthanum zirconate ($\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, LLZO) is a promising solid electrolyte for all-solid-state lithium batteries with improved safety characteristics. However, the different phases of LLZO differ in lithium ionic conductivity by several orders of magnitude, with extrinsic dopants often required to stabilize the high conductivity cubic phase. Here we show that undoped and doped cubic LLZO nanowires can be prepared using electrospinning. Detailed structural characterization with XRD and TEM were performed to understand the LLZO formation processes and phase transformations. The LLZO nanowires were further investigated as ceramic fillers for solid polymer electrolytes. Composite solid electrolytes (CPEs) containing ceramic fillers embedded inside a polymer-salt matrix show great improvements in Li^+ ionic conductivity compared to the polymer electrolyte alone. CPEs with LLZO nanoparticle and Al_2O_3 nanowire fillers were also studied to elucidate the role of filler type, LLZO composition, and morphology on the CPE conductivity. It is demonstrated that both intrinsic Li^+ conductivity and nanowire morphology are needed for optimal performance.

9:00 AM

(EMA-S11-002-2017) The role of interfaces in all solid-state batteries (Invited)

N. J. Taylor^{*1}; Y. Kim¹; T. Thompson¹; J. Sakamoto¹; 1. University of Michigan, USA

Growing energy needs require safer and higher performance batteries than today's state of the art Li-ion batteries. All solid state batteries (ASSBs) have the potential to provide a significant step

forward in Li battery technology. One promising solid state electrolyte is $\text{Li}_{6.25}\text{La}_3\text{Al}_{0.25}\text{Zr}_2\text{O}_{12}$ (LLZO), which has high room temperature ionic conductivity and chemical and mechanical stability towards metallic Li. Sulfide based solid electrolytes have high room temperature conductivities, but poorly defined stability versus metallic Li. In this talk, we describe the role of interfaces in the construction of ASSBs with a metallic Li anode, LLZO electrolyte, and composite cathode consisting of $75\text{Li}_2\text{S}:25\text{P}_2\text{S}_5$ sulfide electrolyte and TiS_2 cathode. In this cell architecture, the LLZO isolates the metallic Li anode and the sulfide based composite cathode is easily fabricated by cold pressing. Hybrid oxide/sulfide cells were cycled at 70°C and the LLZO/ $\text{Li}_2\text{S}:\text{P}_2\text{S}_5$ interface was characterized by electrochemical impedance spectroscopy (EIS). We also discuss the materials chemistry and interfaces of co-sintered LLZO and commercial oxide cathodes in the context of all oxide ASSB cell construction.

9:30 AM

(EMA-S11-003-2017) Structural and Electrochemical Response to Irradiation Induced Defects in TiO_2 Anodes for Lithium-ion Batteries

K. A. Smith^{*1}; D. Butt¹; J. Wharry³; C. Xiong¹; 1. Boise State University, USA; 2. University of Utah, USA; 3. Purdue University, USA

The objective of this study is to understand the effect of irradiation on TiO_2 anodes for electrical energy storage applications. Considering the enhanced electrochemical behavior of electrodes containing intentional structural defects, we hypothesize that nanoscale transition metal oxides with local disorder may offer higher capacity and enhanced stability under electrochemical cycling. In this study, we first focus on separating the effects of irradiating species and crystallographic orientation on defect production by conducting irradiation experiments on rutile TiO_2 single crystals. We then extend our study to investigate the effects of irradiation on nanostructured TiO_2 electrodes.

9:45 AM

(EMA-S11-004-2017) Enabling Next Generation Sodium-Based Batteries with Engineered NaSICON Ion Conductors

E. D. Spoecker^{*1}; L. Small¹; P. Clem¹; J. Lamb¹; E. Allcorn¹; G. Nagasubramanian¹; D. Ingersoll¹; A. Eccleston²; S. Bhavaraju²; 1. Sandia National Laboratories, USA; 2. Ceramtec, Inc., USA

Safe, reliable, low-cost, electrical energy storage is important for the renovation and evolution of the national electric grid. Effective energy storage enables renewable energy integration, agile energy distribution, effective emergency response, and even national defense. Here, I will describe a new generation of sodium-based batteries, enabled by the sodium super ion conductor NaSICON. These systems rely on exceptional low-to-intermediate temperature sodium ion conductivity and excellent chemical stability of this ceramic ion conductor. Integrating NaSICON into all-inorganic battery constructs, we create high performance energy storage systems that operate below 200°C and avoid hazards associated with polymer separators and organic electrolytes used in other batteries. I will describe the design and performance of emerging technologies including Na- NiCl_2 , Na- I_2 , and aqueous Na-based systems, highlighting functional and safety-related benefits of these ceramic-enabled batteries. Finally I will describe recent materials research aimed at resolving challenges that must be met to advance these emerging Na-based technologies. Sandia National Laboratories is a multi-mission laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the US Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Processing and Microstructure Effects on Ion Conduction

Room: Caribbean C

Session Chair: Fanglin (Frank) Chen, University of South Carolina

10:30 AM

(EMA-S11-005-2017) Processing Nanostructured YSZ Scaffolds at High Temperatures via in situ Carbon Templating of Hybrid Materials (Invited)

M. D. Gross^{*1}; 1. Wake Forest University, USA

Porous mixed-metal-oxide scaffolds coated with electrocatalytic particles are often used as electrodes in highly efficient electrochemical devices, including solid oxide fuel cells, electrolyzers, membrane reactors, and gas separators. To improve electrode performance, a large body of research has focused on increasing the surface area of the electrocatalytic particles, but there is little research on increasing the scaffold surface area. Increasing the scaffold surface area is challenging because they are sintered at high temperatures, 1100°C to 1500°C . Here we describe a novel approach to realize porous, nanostructured yttria-stabilized-zirconia (YSZ) scaffolds with specific surface areas up to $80\text{ m}^2/\text{g}^{-1}$; traditionally sintered scaffolds have specific surface areas of $0.1\text{--}1\text{ m}^2$. With this approach, a hybrid inorganic-organic material is sintered in an inert atmosphere producing a mixture of YSZ and amorphous carbon in situ. The carbon serves as a hard template during sintering and is subsequently removed by low temperature oxidation, resulting in a porous, nanostructured YSZ scaffold with high surface area. The method is flexible in that the concentration of carbon template, scaffold surface area, and porosity can all be systematically tuned by controlling the total amount of organic content in the hybrid material.

11:00 AM

(EMA-S11-006-2017) Novel Processing of Composite Cathodes for Proton Ceramic Fuel Cells by Exsolution (Invited)

M. Einarsson^{*1}; L. Rioja-Monllor¹; C. Bernuy-Lopez¹; M. Fontaine²; T. Grande¹; 1. NTNU Norwegian University of Science and Technology, Norway; 2. SINTEF Materials and Chemistry, Norway

This work focuses on development of new composite cathode materials for BaZrO_3 -based proton conducting fuel cells by a novel exsolution method. The cathodes were prepared by in situ oxidation driven decomposition of a single phase precursor described by the following nominal compositions: $\text{La}_{0.3}\text{Ba}_{0.7}\text{Zr}_{0.4}\text{M}_{0.6}\text{O}_{2.75} + \text{O}_2 \rightarrow 0.6\text{La}_{0.5}\text{Ba}_{0.5}\text{MO}_{3-\delta} - 0.4\text{BaZrO}_3$ where M is Mn, Fe and/or Co. The single phase precursor was synthesized by a modified Pechini route optimized in order to obtain an amorphous solid state precursor. The phase composition upon further thermal processing was defined by controlling the oxidation state of cobalt. The precursor was heated at 900°C in air in order to achieve a composite consisting of a $\text{La}_{1-x}\text{Ba}_x\text{CoO}_{3-\delta}$ - and a BaZrO_3 -based material. In situ HT-XRD in air enabled to identify the formation mechanisms of the composites. For example the single phase precursor with $\text{M}=\text{Co}$ formed in reducing atmosphere was exsolved into the composite " $\text{La}_{1-x}\text{Ba}_x\text{CoO}_{3-\delta} - \text{BaZrO}_3$ " at $\sim 800^\circ\text{C}$. Characterization of the exsolved composites includes electrical conductivity, microstructure and electrochemical properties by impedance spectroscopy. Electrochemical characterization as cathodes in symmetrical cells shows promising results. A discussion of the electrochemical characterization of the composite materials as a cathode for PCFC will be presented with the focus on the effect of varying M.

S15: Superconducting Materials and Applications

Advances in Carbon Conductors: Physics and Applications

Room: Pacific

Session Chairs: Timothy Haugan, U.S. Air Force Research Laboratory; Judy Wu, University of Kansas

8:30 AM

(EMA-S15-027-2017) Will carbon nanotube based wires transform the field of electrical machines? (Invited)

A. E. Lekawa-Raus^{*1}; 1. Warsaw University of Technology, Poland

Back in 2013 our Cambridge (UK) group has presented the first in the world electrical machines (transformers, generators, motors) in which all standard copper windings were replaced with wires made of carbon nanotube (CNT) fibres i.e. long thin assemblies of axially aligned nanotubes. Soon, this field has been entered by other research groups as the CNT wires are believed to have a potential to decrease the weight of machines, improve their efficiency or rotation speed. Unfortunately, up to now all the CNT wound machines have very poor performance as currently produced CNT fibres are not sufficiently conductive. Basic research in individual CNTs backed up by scientific intuition indicates the methods of improvement of CNT fibre conductivity e.g. via increase in length of CNTs, removal of defects and impurities or improvement of alignment. But do we know what the electrical performance perfectly structured CNT fibres will be like? Our recent study shows that not necessarily. Moreover, there may not be only one perfect structure, but it may depend on the application of our wires.

9:00 AM

(EMA-S15-028-2017) Magneto-transport of highly graphitic, highly aligned carbon nanotube fibers (Invited)

J. Bulmer^{*1}; 1. Cambridge University, United Kingdom

A multistep photonic-enabled post-process transforms partly aligned carbon nanotube (CNT) textiles to highly aligned, highly graphitic CNT fiber of substantially greater conductivity. Cryogenic, magnetic field dependent transport characterization shows different transport responses for both materials. Both materials are on the metal side of the insulator to metal transition. Negative magneto-resistance is explained by weak localization. For the as-is material, weak localization is two dimensional indicating the limiting influence of CNT bundles. For the photonic treated material, weak localization is three dimensional indicating bundle junctions have less influence. At higher field, positive magneto-resistance is present and is shown to be classical in nature. This enables measurement of the CNT fiber's charge carrier mobility, which is useful for quality control. For both materials, most of the room temperature resistance comes from the fluctuation induced tunneling mechanism. Evidence indicates this mechanism has no magneto-resistance, which seems to be an open question in literature.

9:30 AM

(EMA-S15-029-2017) An examination of the evidence for superconductivity in doped graphite and graphene (Invited)

G. Larkins^{*1}; Y. Vlasov²; K. Holland¹; 1. Florida International University, USA; 2. Florida International University, USA

We have observed evidence at temperatures in the vicinity of 260 K of superconductivity in phosphorous doped graphite and graphene. This includes transport current, magnetic susceptibility, Hall Effect and (pancake) vortex state measurements. All of these measurements indicate a transition that is that of a type II superconductor with no type I phase until below the limits of our measurement capabilities. These results will be discussed in detail. In addition

we have also examined a number of other dopants, including boron, aluminum, arsenic, fluorine, lithium, nitrogen, sodium and sulfur in graphene and Highly Oriented Pyrolytic Graphite. The results of these studies will be presented and discussed in the context of the more widely published results using phosphorous as a dopant in graphene and Highly Oriented Pyrolytic Graphite.

10:30 AM

(EMA-S15-030-2017) Development and Measurement of Carbon Nanotube-metal composite conductors (Invited)

M. Sumption^{*1}; 1. The Ohio State University, USA

There is a significant opportunity for the development of CNT-metal composites with high electrical and thermal conductivity, as well as high current density. Such conductors, aiming at high conductivity and/or high conductivity per unit weight, have potential applications in electronics, transportation, and high power density applications. In this work, we discuss the development of CNT/metal composites based on powder in tube, electrochemical metallization, and co-deposition approaches. Our composites are formed with Cu and Al metals, and various CNT and graphene additions. Functionalization both during and after composite fabrication are discussed. A particularly promising approach appears to be the encapsulation and functionalization of CNT yarns. We have measured both electrical and thermal conductivity in the temperature range from room temperature to 400C, as well as conductor ampacity. Absolute as well as mass-normalized electrical and thermal conductivity results are discussed, and it is seen that results on a mass based basis are already of potential application interest for some composites.

11:00 AM

(EMA-S15-031-2017) Hints of superconductivity in graphitic materials (Invited)

N. Gheorghiu^{*2}; C. B. Ebbing⁴; M. Sumption³; T. J. Haugan¹; 1. Air Force Research Laboratory, USA; 2. UES, Inc., USA; 3. Ohio State University, USA; 4. University of Dayton Research Institute, USA

Hints of superconductivity in graphitic materials There are reports on: superconductivity in graphite treated with either alkanes or water; super-acidic protons produced on the graphite surface in contact with alkanes moving freely without activation energy; ferromagnetism in proton irradiated graphite; ferromagnetism and superconductivity coexistence in some magnetic materials. Our studies are looking into the alkanes' effect on graphitic samples. PPMS measurements used the DC Resistivity and VSM options to obtain magnetoresistance and magnetization data on carbon fibers and pyrolytic graphite, as-are or treated with alkanes. Temperatures ranged from 1.9 or 5 K to 300 K and magnetic fields up to 9 T were applied. At 1.9 K, magnetoresistance loops show anomalous hysteresis, observed by others for conventional and high-temperature superconductors, as well as for graphite flakes and also at graphite interfaces. At 5 K and 9 K, the hysteresis is normal, observed by others for bulk superconductors with pinned Abrikosov flux lines and also for ferromagnets. VSM measurements on pyrolytic graphite found abrupt changes in the temperature-dependent magnetization M(T) curve, with ferromagnetic, paramagnetic, and diamagnetic phases. The latter appears at ~ 150 K, also found by others as the mean-field critical temperature for a Cooper-like pairing instability. Could ferromagnetism hinder superconductivity in this case?

11:30 AM

(EMA-S15-032-2017) Synthesis and physical properties of new iron-based compound EuFeAs₂

H. Ogino^{*1}; A. Sala¹; H. Tanaka²; K. Kishio²; Y. Goto¹; A. Iyo¹; H. Eisaki¹; 1. National Institute of Advanced Industrial Science and Technology, Japan; 2. University of Tokyo, Japan

Since 2008, series of iron-based superconductors have been developed. Recently new iron-based superconductor (Ca,RE)FeAs₂ was

discovered. The compounds show superconductivity above 40 K. Crystal structure of the $(\text{Ca,RE})\text{FeAs}_2$ is composed of Fe_2As_2 layer, $\text{Ca}(\text{RE})$ plane, and As_2 layer. In As_2 layer, closest As-As distance is ~ 2.60 Å, suggesting existence of two As-As bonding for each As atom, which is the first example in iron-based superconductors. Anisotropy of the compound is lower than that of REFeAsO , though distance between superconducting layers of this compound is longer than that of REFeAsO . We have explored relative compounds of $(\text{Ca,RE})\text{FeAs}_2$ and discovered new iron-based superconductor EuFeAs_2 . The compound also contains As_2 chain which is similar to that of $(\text{Ca,RE})\text{FeAs}_2$. Zero resistivity was observed above 10 K. Synthesis and physical properties of the compound will be presented.

S1: Advanced Electronic Materials: Processing, Structures, Properties, and Applications

Characterization of Materials: Crystal Structure and Properties II

Room: Indian

Session Chair: Matthew Cabral, North Carolina State University

2:00 PM

(EMA-S1-056-2017) Use of Bayesian Inference in Characterization of Ceramic Materials: An Introduction and Applications in Ferroelectrics (Invited)

J. L. Jones^{*1}; J. Guerrier¹; T. Iamsasri¹; C. Fancher¹; J. E. Daniels²; A. Larsen³; A. Wilson³; B. Reich³; R. Smith¹; 1. North Carolina State University, USA; 2. University of New South Wales, Australia; 3. North Carolina State University, USA; 4. North Carolina State University, USA

Materials development remains limited by our ability to “see” and characterize newly synthesized materials. Over the past decades, great advancements have been seen in X-ray and neutron characterization instruments. However, the analysis of data from such instruments has progressed slowly, an example being the Rietveld method for refinement of crystallographic structures using least squares (1969). In this talk, I will introduce to the materials researcher the alternative statistical framework of Bayesian statistics and its application to analysis of diffraction data when employed in conjunction with a Markov Chain Monte Carlo (MCMC) algorithm. The talk will include a basic introduction and application to modeling single reflections, doublets from ferroelastic degenerate reflections, and the entire pattern (full profile). The parameters in the new models represent structure using probability distributions, treating solutions probabilistically with improved uncertainty quantification. For ferroelectrics, we demonstrate that these probability distributions can be readily propagated into new calculated parameters related to domain reorientation. The conventional least squares solutions and its confidence intervals will be compared/contrasted to the new approach and its credible intervals. The new approach offers more confident structure-property correlations.

2:30 PM

(EMA-S1-057-2017) Structural and Thermal Characterization of the $\text{Mg}_x\text{Co}_x\text{Cu}_x\text{Ni}_x\text{Zn}_x\text{O}$ $x=0.2$ Entropy Stabilized Oxide

C. M. Rost^{*2}; J. Braun²; P. Hopkins²; J. Maria¹; 1. North Carolina State University, USA; 2. University of Virginia, USA

Entropy-stabilized oxides (ESOs) demonstrate the viability of materials engineering where configurational entropy drives phase stabilization. Here, we present the application and analysis of extended x-ray absorption fine structure (EXAFS) on the prototype ESO composition $\text{Mg}_x\text{Ni}_x\text{Co}_x\text{Cu}_x\text{Zn}_x\text{O}$ ($x = 0.2$). We find that local bond lengths between metal and oxygen vary around each absorbing cation, with notable distortion around the Cu-O polyhedra. By the

second coordination shell, interatomic distances are uniform within our resolution limits. Structural models that best fit the experimental scattering data include cations that are distributed randomly on an FCC sublattice with minimal positional disorder, with an interleaved FCC anion sublattice with oxygen ions displaced from the ideal locations to accommodate the distortions in the cation polyhedra. Using time domain thermoreflectance (TDTR), we measure the thermal conductivity of the prototype ESO for comparison with other, less disordered compositions containing the same constituents. We find thermal conductivity to systematically lower with increasing configurational disorder. Changes in thermal conductivities are discussed in terms of the various scattering mechanisms at play with an emphasis of understanding such mechanisms from a local structural perspective.

2:45 PM

(EMA-S1-058-2017) Structure-property-processing relationships in $\text{BiScO}_3 - \text{PbTiO}_3$

B. Kowalski^{*1}; A. Schirlioglu¹; 1. Case Western Reserve University, USA

In recent years there has been an intense push for high temperature piezoelectrics for applications in both terrestrial and aerospace territories. For years the operating temperature limit, usually taken as $\frac{1}{2}$ the Curie temperature (T_c), has been $\sim 200^\circ\text{C}$ for one of the most widely used commercial piezoelectrics, $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT). Subsequent research into $\text{Bi}(\text{B}'\text{B}'')\text{O}_3 - \text{PbTiO}_3$ piezoelectrics led to the discovery of the morphotropic phase boundary (MPB), high- T_c system $\text{BiScO}_3 - \text{PbTiO}_3$ (BS-PT) with a T_c of 460°C and a d_{33} of 460 pm/V. While the T_c marks the boundary between the ferroelectric-paraelectric state, it is also necessary to determine the depoling temperature (T_d) which dictates the actual working temperature range. This work will investigate thermal depoling in rhombohedral, tetragonal, and mixed phase compositions around the MPB in BS-PT. Impedance analysis will be used to show that thermal depoling occurs over a temperature range, rather than as a single temperature. Thermal stability will be investigated further through isothermal impedance analysis over time. Also, high temperature X-ray diffraction will be employed to connect the impedance analysis to structure/strain changes in the material.

3:00 PM

(EMA-S1-059-2017) Structural and Electrical Properties of PZN-PZT Piezoceramic Fibers with Low Sintering Temperature and Their Device Applications

E. Mensur-Alkoy^{*2}; M. Y. Kaya¹; S. Alkoy¹; 1. Gebze Technical University, Turkey; 2. Maltepe University, Turkey

The relaxor based ternary systems of lead zinc niobate and lead zirconate titanate (PZN-PZT) have recently been investigated for actuator, transducer and sensor applications due to the ease in tailoring electrical properties compared to the PZT binary systems. In this study, $(x)\text{PZN}-(1-x)\text{PZT}$ ceramics were prepared at 950°C sintering temperature with PZN ratios of $x=0.4, 0.5$ and 0.6 . The $0.4\text{PZN}-0.6\text{PZT}$ composition was found to crystallize in perovskite phase at this sintering temperature without the presence of any other secondary phases. Dielectric constant, piezoelectric charge coefficient, electromechanical coupling coefficient and mechanical quality factor of $0.4\text{PZN}-0.6\text{PZT}$ were found as 2608, 477 pC/N, 64.4 and 65, respectively. PZN-PZT fibers with full and hollow circular cross-section were drawn using alginate gelation method. Fibers were obtained after sintering process and piezocomposites were prepared with 1-3 connectivity using full fibers and hollow fibers were investigated for single fiber based active devices. In summary, fiber based transducer devices have successfully been prepared and characterized. The authors acknowledge the financial support by the Scientific and Technical Research Council of Turkey (Project #112M791) and by the Turkish Academy of Sciences through the GEBIP Program.

3:15 PM

(EMA-S1-060-2017) Point defect chemistry and its effect on the order-disorder phase transition and dielectric properties of $\text{Ba}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3$ complex perovskites

A. Sayyadishahraki^{*1}; E. Taheri-Nassaj¹; T. Kolodiazhnyi²; J. Gonzales³; N. Newman³; 1. Tarbiat Modares University, Islamic Republic of Iran; 2. National Institute for Materials Science, Japan; 3. Arizona State University, USA

We report on the effects of non-stoichiometry formation on the point defect chemistry, B site cation ordering and microwave dielectric properties of $\text{Ba}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3$ (BCN) compound. Non-stoichiometric samples with compositions along 11 different tie lines in the $\text{BaO-CoO-Nb}_2\text{O}_5$ ternary diagram were prepared by solid state route and sintered at 1400-1550°C for 10 h to obtain high density bodies. Microwave dielectric measurements showed that the non-stoichiometry formation has a significant effect on the quality factor (inversion of loss tangent) where the samples with compositions along the BCN- $\text{BaNb}_{4/5}\text{O}_3$ tie line possessed quality factors approximately two times that of stoichiometric sample. X-ray diffraction technique was used to determine solubility limit of point defects around stoichiometric BCN compound and the results showed that BCN could only accommodate limited amounts of point defects; however this small solid solubility limit of point defects has a pronounced effect on crystal structure, B site cation arrangement and microwave dielectric loss factor. Rietveld Refinement was employed to calculate Co and Nb cations ordering degree in the octahedral sites of crystal structure. The highest sample (71,000 GHz) with 0.94 BCN- 0.06 $\text{BaNb}_{4/5}\text{O}_3$ composition was identified to have full B site 1:2 cation ordering for Co and Nb ions.

Lead Free Piezoelectrics III

Room: Coral B

Session Chairs: Ken-ichi Kakimoto, Nagoya Institute of Technology; Jiagang Wu, Sichuan University

2:00 PM

(EMA-S1-061-2017) Engineering of Alkali Niobate Piezoceramics and Energy-Harvesting Application (Invited)

K. Kakimoto^{*1}; 1. Nagoya Institute of Technology, Japan

Current interests are focused to well-designed processing and microstructure control of $(\text{Na,K})\text{NbO}_3$ (NKN)-based alkali niobate system; however, literatures on the grain-size-related properties of NKN-series ceramics have remained essentially insufficient to date, although this is a crucial subject for the further improvement of piezoelectric properties. Therefore, the influence of differences in raw Nb-source powder on the sinterability and grain-size-oriented piezoelectric properties is commented; then, an example of a piezoelectric-particle dispersed polymer-based layer-by-layer composite are remarked for a possibility to future application such as a vibration-oriented energy harvester.

2:30 PM

(EMA-S1-062-2017) Relationship between Phase Boundaries and Piezoelectricity in Potassium-Sodium Niobate Lead-free Ceramics (Invited)

J. Wu^{*1}; 1. Sichuan University, China

The construction of phase boundaries is an effective way to promote the piezoelectric activity of potassium-sodium niobate lead-free materials. Here we attained a large piezoelectricity in $(\text{K,Na})\text{NbO}_3$ by constructing different phase boundaries (e.g., R-O, O-T, and R-T). A large piezoelectric coefficient ($d_{33}=350\sim490$ pC/N) was achieved by forming the R-T phase boundary, which is the highest values reported so far in potassium-sodium niobate, suggesting that such a system is a promising lead-free candidate for electromechanical actuator applications. In addition, the underlying physical mechanisms for enhanced electrical properties have been addressed.

We believe that the summative researches can point out the direction for further developing potassium-sodium niobate lead-free materials.

3:00 PM

(EMA-S1-063-2017) Potassium-sodium Niobate (KNN) Based Piezoelectric Ceramic Coatings Derived from Thermal Spray Process

S. Chen^{*1}; C. Tan¹; K. Yao¹; 1. Institute of Materials Research and Engineering (IMRE) Singapore, Singapore

Thermal spray process is well established in industry for fabricating wear and corrosion resistant barrier ceramic coatings. It has many advantages such as high throughput, large area and wide thickness range. However, piezoelectric ceramic coating useful for practical applications have not been produced. Recently, our group has demonstrated the fabrication of potassium sodium niobate (KNN) based lead-free piezoelectric ceramic coatings by thermal spray process. The coatings exhibited single perovskite phase, dense morphology and large piezoelectric coefficient. The effective d_{33} coefficient measured over macroscopic area using laser scanning method reached 112 pm/V under the substrate clamping condition. The reasons for obtaining single-phase perovskite structure and excellent piezoelectric properties in KNN coatings by thermal spray are discussed, in contrast to the processing issues reported in the literature about thermal sprayed lead zirconate titanate (PZT) coatings, based on the analyses on the different characteristics between KNN and PZT compositions, and the reaction mechanisms involved in thermal spray process and solid state synthesis.

3:15 PM

(EMA-S1-053-2017) Fracture toughness of $(1-x)(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3$ - $x\text{BaTiO}_3$ relaxor ferroelectrics

M. Vögler^{*1}; S. M. Denkhau¹; J. Rödel¹; K. G. Webber²; 1. Technical University Darmstadt, Germany; 2. Friedrich-Alexander-University Erlangen-Neurnberg, Germany

Ferroelectrics based on the lead-free $(1-x)(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3$ - $x\text{BaTiO}_3$ (BNT- $x\text{BT}$) system have attracted special interest because of the observed intriguing and extraordinary dielectric and electromechanical properties. The fracture behavior of these new ferroelectric ceramics is often overlooked by the scientific community, even though it is crucial to understand the physical mechanisms of fracture in order to make life cycle predictions and reliability analysis within the design process of new applications. The literature on the fracture mechanics of relaxor ferroelectrics is quite scarce, leaving a gap of knowledge in this field. Our work is based on surface crack in flexure experiments and determined the temperature dependency as well as the effect of poling on the fracture toughness of three compositions ($x = 3, 6, 12$ mol%). This reveals insight into the structure-dependent toughening mechanisms of the BNT- $x\text{BT}$ system. Experimental results are contrasted to a theoretical model, predicting the fracture toughness by taking crystal structure, mechanical hysteresis behavior and Young's modulus into account. Our results show a decrease in fracture toughness with temperature and an increase upon poling. The shielding effect is found to be very low in comparison to other ferroelectrics, mainly due to the high coercive stress, which limits ferroelastic toughening to a very narrow region around the crack tip.

Lead Free Piezoelectrics/Ferroelectric Superlattice

Room: Coral B

Session Chair: Xiaoli Tan, Iowa State Univ

4:00 PM

(EMA-S1-065-2017) Low Temperature Sintering, Atmospheric Control, and Bismuth Deficiency in Morphotropic Phase Boundary BNT-BKT-BT Ceramics

G. Yesner^{*1}; A. Safari¹; I. Rutgers University, USA

Bi-based piezoelectric ceramics are a good candidate to replace lead zirconate titanate (PZT). One of the applications of lead zirconate titanate (PZT) is the use in multilayer actuators (MLA) for diesel fuel injectors. Currently, state of the art fuel injectors utilize PZT multilayer actuators with internal copper electrodes. PZT with copper metal electrodes must be co-fired at a low temperature and under a controlled atmosphere. Bi-based ceramics can be co-fired with Cu, but the range of oxygen partial pressure Cu metal and Bi₂O₃ is extremely narrow compared to PbO. In this work 0.88Bi_{1/2}Na_{1/2}TiO₃ - 0.08Bi_{1/2}K_{1/2}TiO₃ - 0.04BaTiO₃ (BNT-BKT-BT) ceramics have been sintered at 900°C in controlled atmosphere. Sintering at 900°C is accomplished using a combination of sintering aids. The ceramics are sintered under an oxygen partial pressure of 6.1×10^{-8} atm. The room temperature piezoelectric properties of BNT-BKT-BT sintered at 900°C in controlled atmosphere are similar to BNT-BKT-BT sintered at 1150°C. Additional study was given to the effect of non-stoichiometry of A-site cations in BNT-BKT-BT. Hardening and softening of piezoelectric properties has been observed. The most notable effect is that the mechanical quality factor of the Bi-deficient composition is as high at 1200 compared to 150 for the unmodified composition.

4:15 PM

(EMA-S1-066-2017) Effect of Sr²⁺ Doping on the Structural and Electrical Properties of Bi(Na,K)TiO₃ Lead-Free Ceramics

V. Kalem^{*1}; 1. Selcuk University, Turkey

Polycrystalline $(1-x)[0.8\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3 - 0.2\text{Bi}_{0.5}\text{K}_{0.5}\text{TiO}_3] - (x)[\text{SrTiO}_3]$ ($x = 0$ to 0.20) lead-free piezoelectric ceramics were synthesized via a solid-state reaction route. Microstructural and compositional analyses have been carried out using X-ray diffraction (XRD) and scanning electron microscope (SEM). XRD patterns indicated that undoped composition ($x = 0$) had a tetragonal phase dominant structure, however SrTiO₃ (ST) incorporations resulted in a phase shift to rhombohedral symmetry. SEM studies showed that increasing ST doping led to a decrease in grain size. Effect of ST doping on the piezoelectric and dielectric properties were also investigated. The results revealed that the dielectric constant increased gradually with the increase of ST. The ceramic having 12 mol% ST possessed the optimum properties ($d_{33} = 205$ pC/N, $k_p = 0.36$, $K^T = 1520$, $\tan\delta = 6.1\%$, $Q_m = 87$, $T_m = 285^\circ\text{C}$) enabling this composition a suitable lead-free candidate for piezoelectric actuator applications.

4:30 PM

(EMA-S1-067-2017) The role of interfaces on strain-enabled ferroelectricity in CaTiO₃/SrTiO₃ superlattices (Invited)

R. Engel-Herbert^{*1}; 1. Pennsylvania State University, USA

Research of layered complex perovskite oxide superlattices has received considerable attention in recent years, as these artificial structures can possess properties that are beyond the bulk counterparts of the constituting layers. The emergence of these otherwise unattainable properties have been attributed to the presence of interfaces and the overwhelming majority of reported results in literature have suggested that atomically sharp interfaces are a mandatory requirement for these novel phenomena to emerge. The commonly accepted and intuitive notion is that strength and stability of the emergent property is proportional to the interface density and thus inversely proportional to the layer number n in the perovskite superlattice structure. In this talk the role of stoichiometry on stabilizing

the ferroelectric ground state in strained CaTiO₃ and SrTiO₃ thin films as well as (CaTiO₃) _{n} (SrTiO₃) _{n} superlattices is discussed. Their analysis for layering thicknesses ranging from $n=1$ to 10 unit cells revealed that the ferroelectric properties were dependent on the layer thickness fluctuation Δn , rather than on the layer thickness n . Ferroelectricity was only observed for $\Delta n > 0.1$ irrespective of n , suggesting the critical role of layer uniformity on emerging properties in functional oxide superlattices.

S3: Ceramic Photonic Materials and Applications

Ceramic Photonic Materials and Applications II

Room: Mediterranean C

Session Chairs: Haiyan Wang, Purdue University; Yoshio Bando, National Institute for Materials Science (NIMS)

2:00 PM

(EMA-S3-008-2017) Novel synthesis and analysis of BN nanotube/nanosheet and applications (Invited)

Y. Bando^{*1}; 1. National Institute for Materials Science (NIMS), Japan

Boron nitride (BN) materials are attracting more and more attentions due to their constant and wide band gap independent of morphology, superb mechanical properties, very high thermal conductivity and marked chemical inertness. Recently, we have developed novel methods for synthesis of large scale highly pure BN nanotubes and nanosheets. Thinner BN nanotubes with diameter smaller than 10 nm were fabricated successfully. Large scale BN nanosheets were also fabricated by the "chemical blowing method". Subsequently, boron nitride polymeric composites were fabricated and their thermal, electrical and mechanical properties were evaluated. More than 20-fold thermal conductivity improvement was achieved, and such composites keep good electrical insulation. In addition, in situ mechanical and electrical properties from individual BN nanotubes and nanosheets have been successfully studied under the TEMs using STM/AFM-TEM special holders. The Young modulus of BN nanotube was observed to be 0.9TPa, which is comparable with carbon nanotube.

2:30 PM

(EMA-S3-009-2017) Self-Assembled Epitaxial Au-Oxide Vertically Aligned Nanocomposites for Nanoscale Metamaterials (Invited)

L. Li^{*1}; L. Sun²; J. Sebastian Gomez-Diaz²; N. L. Hogan¹; P. Lu³; F. Khatkhatay¹; W. Zhang¹; J. Jian¹; J. Huang¹; Q. Su¹; M. Fan¹; C. Jacob¹; X. Zhang⁴; Q. Jia⁵; M. Sheldon¹; A. Alù²; X. Li²; H. Wang¹; 1. Texas A&M University, USA; 2. The University of Texas at Austin, USA; 3. Sandia National Laboratories, USA; 4. Purdue University, USA; 5. Los Alamos National Laboratory, USA

Metamaterials made of nanoscale inclusions or artificial unit cells exhibit exotic optical properties that do not exist in natural materials. Promising applications such as cloaking and hyperbolic propagation have been demonstrated based on mostly micrometer-scale metamaterials and few nanoscale metamaterials. To date, most metamaterials are created using costly and tedious fabrication techniques. Here, we demonstrate the one-step direct growth of self-assembled epitaxial metal-oxide nanocomposites as a drastically different approach to fabricating large-area nanostructured metamaterials. Using pulsed laser deposition, we fabricated nanocomposite films with vertically aligned Au nanopillars embedded in various oxide matrices. Strong, broad absorption features in the measured absorbance spectrum are clear signatures of plasmon resonances of Au nanopillars. By tuning their densities on selected substrates, anisotropic optical properties are demonstrated via angular dependent and polarization resolved reflectivity measurements and reproduced by full-wave simulations and effective medium theory. Our model predicts exotic properties,

such as zero permittivity responses and topological transitions. Our studies suggest that these self-assembled metal-oxide nanostructures provide an exciting new material platform to control and enhance optical response at nanometer scales.

3:00 PM

(EMA-S3-011-2017) The tailoring of microstructure of percolative composites for RF metamaterials (Invited)

R. Fan^{*1}; 1. Shanghai Maritime University, China

Metal-ceramic composites with three-dimensional metallic networks hosted in porous ceramic matrix were prepared by a facile impregnation process under low temperature. The effects of composition and microstructure on their electromagnetic properties were investigated. A percolation phenomenon appeared with metal content increasing, and an interesting feature of negative permittivity was obtained in the percolative composites due to the appearance of equivalent inductances, while the composites were equivalent to circuit models composed of capacitance and resistance with metal content below the percolation threshold. Meanwhile, negative permeability was obtained in the RF frequency. That was to say, double negative properties of typical metamaterials could be tailored by compositions and microstructures of metal-ceramic composites, which make it available for microwave-absorbing materials, attenuation ceramics and microwave dielectrics, etc.

4:00 PM

(EMA-S3-012-2017) Field-assisted solid-state single crystal conversion (Invited)

Y. Liu^{*1}; Y. Wu¹; 1. New York State College of Ceramics, Alfred University, USA

The solid-state single crystal conversion of an isotropic (CaF_2) and anisotropic ceramic ($\text{Sr}_5(\text{PO}_4)_3\text{F}$) were studied. A DC electric field was introduced to facilitate densification and seed crystal growth. The seed crystal was bonded to the ceramic, and it was observed that crystal growth increased with increasing heat treatment time. Electric field application was demonstrated to be effective in enhancing densification and restraining grain growth. The relative ratios of grain growth to crystal growth were also studied to show the close interrelation between the two factors regardless of the solid-state processing conditions, which implies that within the normal grain growth regime, the degree of seed crystal growth increases with the growth of the polycrystalline grains. This phenomenon is conjectured to be the main cause for the limited degree of crystal growth obtained using the solid-state conversion method.

S4: Computational Design of Electronic Materials

Low-Dimensional Structures

Room: Coral A

Session Chair: Lan (Samantha) Li, Boise State University

2:00 PM

(EMA-S4-028-2017) Thermal Conductivity Modeling of Hybrid Organic-Inorganic Crystals and Superlattices (Invited)

R. Yang^{*1}; X. Qian¹; X. Gu¹; 1. University of Colorado, USA

There has been growing interest in hybrid organic-inorganic materials, which can combine the superior properties of both components, such as the good electronic properties from inorganic materials and the superb flexibility from organic materials. Furthermore, the thermal conductivity of hybrid materials can be reduced due to the heterogeneous bonding and interfaces. As such, we witness significant efforts in developing flexible thermoelectrics using hybrid materials. However, the thermal conductivity of organic-inorganic hybrid crystals and superlattices is rarely studied. Even though first-principles-based calculations are increasingly used to

predict thermal conductivity of inorganic crystals. It is challenging to use the conventional first-principles calculations to predict the thermal conductivity of hybrid materials due to the complexity of crystal structures and computational costs. In this talk, we discuss our efforts in developing the first-principles-based atomistic simulation methodology to predict thermal conductivity of hybrid crystals and superlattices. The phonon transport mechanisms in some novel hybrid crystals, such as hybrid $\beta\text{-ZnTe}(\text{en})_{0.5}$ and hybrid perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$, are discussed. We also present the challenges in modeling the thermal conductivity of hybrid superlattices of organic-intercalated TiS_2 .

2:30 PM

(EMA-S4-029-2017) Ab-initio Design of Oxides for Non-Volatile Memory (Invited)

D. Stewart^{*1}; 1. HGST, A Western Digital Company, USA

Key physical limitations in existing memory technologies are forcing researchers to explore alternative approaches in an effort to maintain Moore's law. Non-volatile resistive RAM memory based on transition metal oxides offers one potential route to circumvent the problems at small scales that have plagued traditional memory devices (DRAM, SRAM, and Flash). In transition metal oxides, a sufficiently large applied field can lead to the formation of a conductive vacancy filament and a low resistance ON state. This conductive filament can also be destroyed using an appropriate applied bias to restore the high resistance OFF state. Given that this memory switching phenomena involves both ionic motion and electronic transport, the details of this process have been difficult to resolve and optimize. Ab-initio calculations can provide critical insight into the defect formation and diffusion necessary to create and break conductive pathways. I will discuss our recent work using different material combinations and dopants to optimize vacancy formation and diffusion in key RRAM oxides (HfO_2 , Ta_2O_5). We search through a broad range of dopants from the periodic table and find clear trends due to dopant valence charge and orbital character. I will also discuss how atomic disorder, electrode material and interface layers can affect vacancy dynamics, electronic transport, and device performance.

3:00 PM

(EMA-S4-030-2017) Neutron scattering studies of organic-inorganic photovoltaic perovskites (Invited)

S. Lee^{*1}; 1. University of Virginia, USA

The record solar cell efficiency based on hybrid organic-inorganic perovskites (HOIPs) has reached 22% which rivals that of conventional silicon solar cells. Combined with its inexpensive solution based processing and all earth abundant compositions, HOIPs are among the most promising next generation solar cell materials. A challenge for hybrid perovskite solar cells is device instability, which calls for understanding of the perovskite structural stability and phase transitions. In this talk, I will present our recent studies, using elastic and inelastic neutron scattering, and ab initio calculations, on two HOIPs, methylammonium lead iodide and formamidinium lead iodide, to understand the perovskite structural stability and phase transitions. We also show that rotational modes of the organic cations are intimately linked to the photovoltaic effects.

3:45 PM

(EMA-S4-031-2017) Magnetic anisotropy in two dimensional transition metal nitrides

J. J. Gabriel^{*1}; D. Stewart²; R. G. Hennig¹; 1. University of Florida, USA; 2. HGST, USA

Two dimensional materials are notable for their unique magnetic and electronic properties that are controlled by changes in structure or composition. Recently, computational studies have shown that two dimensional materials can be promising candidates for

^{*}Denotes Presenter

spintronic applications, because of semiconducting behavior and anisotropies in the magnetic moment. We determine the electronic and magnetic properties of the new family of 2D transition metal nitrides MN_2 ($M = Cr, Mo, W, V, Mn, Nb, Fe$) in the 1T and 2H structures and various distortions with density-functional theory and our open source high-throughput framework MPInterfaces. We calculate their thermodynamic stability relative to known bulk phases, the electronic band structure, the origin of the magnetic moments and the magnetic anisotropy energy. Among the transition metal nitrides we find that Cr, Mo, W nitrides exhibit sizable magnetic moments of more than 1 Bohr per transition metal atom. We identify factors that induce the magnetic anisotropy in this family of two dimensional materials from the features of composition, the orbital origin of the magnetic moment and the structural distortions in these new two dimensional materials.

4:00 PM

(EMA-S4-032-2017) Nanoscale Investigation of Ferroelectric Response of Nanostructures through Molecular Dynamics Simulation

M. Li^{*1}; X. Zeng²; L. Lin²; R. Guo¹; A. Bhalla¹; 1. University of Texas at San Antonio, USA; 2. University of Texas at San Antonio, USA

Due to a wide range of potential industrial application of ferroelectric nanostructures, intensive experimental and computational efforts have been made recently to understand the ferroelectric response of ferroelectric nanostructures. Moreover, the ferroelectric nanostructures are critical in light of miniaturizing piezoelectric transducers and actuators, ultrasonic devices, and medical imaging detectors. However, the ferroelectric response of ferroelectric nanostructures remains unclear until now. To further elucidate the relation of property and performance of ferroelectric nanostructures, this study aims to investigate the ferroelectric response of ferroelectric nanostructures under electric, magnetic, temperature and mechanical fields through molecular dynamics simulation. In this study, the deformation process and the ferroelectric response of ferroelectric nanostructures were investigated. Furthermore, the strain-stress relationship was also obtained through the simulation.

4:15 PM

(EMA-S4-033-2017) Shape of nanocrystals of transition metal oxides predicted in vacuum and in solvent

V. Kolluru^{*1}; R. G. Hennig¹; 1. University of Florida, USA

We predict the shape of MnO , FeO , NiO and CoO nanocrystals in vacuum and in water, by calculating the surface energies of the (100), (110), and (111) facets of these compounds in respective environments and performing the Wulff construction. For the (111) facet, we consider various reconstructions that remove the polar nature of the unreconstructed surface. To match the observed magnetic order and the experimental band gaps of the room temperature phases, we perform density-functional calculations including a Hubbard-U (DFT+U) for the d-electrons of the transition metal atoms. We calculate the surface energies in each system using the DFT+U method and compare it with PBE non-magnetic calculations, to show the importance of including the effects of correlation and exchange. In case of MnO , FeO and CoO – which are paramagnetic semiconductors or insulators at room temperature, we model the random local spin moments using quasi-random structures. The processing conditions of these oxide nanoparticles, in most cases, involves a solvent. To analyze the influence of the solvent environment on the surface energies of different planes and thereby the crystal shape, we calculate the surface energies of these oxides in water using the continuum solvent model VASPsol. We find that the surface energy decreases by different fraction for different facets, affecting the resulting shape of the nanocrystals.

4:30 PM

(EMA-S4-034-2017) Discovery of Transition-Metal Halide Monolayers and the Characterization of their Magnetic and Electronic Properties

J. T. Paul^{*1}; M. Ashton¹; J. J. Gabriel¹; R. G. Hennig¹; 1. University of Florida, USA

Single-layer materials present a new class of materials that have the potential to create innovative solutions to problems in nanoelectronics and energy applications. To accelerate the discovery of these materials, we developed a high-throughput approach – based on our Python package MPInterfaces and density functional theory – that utilized periodic trends and explores chemical substitutions for known 2D structures to identify potentially stable 2D materials. We apply the approach to explore the family of 2D transition metal halides. Performing chemical substitutions for 10 unique monolayer prototype structures, we determine the most stable structure among the 120 possible transition metal halides. We discover over 80 feasible monolayers with formation energies comparable to already extant 2D materials. We calculate the electronic properties, such as the band gap, band edge alignment, and work function, and the magnetic structure of the 2D transition metal halide compounds. We find more than 25 compounds with magnetic moments over 1 Bohr, indicating their potential use in spintronics applications.

4:45 PM

(EMA-S4-035-2017) First-Principles and Grand Canonical Monte Carlo Simulations of Electrochemical Response of Pseudocapacitive β - MnO_2 Electrodes

Y. Okada^{*1}; N. Keilbart²; I. Dabo²; S. Higai¹; K. Shiratsuyu¹; 1. Murata Manufacturing Co., Ltd., Japan; 2. The Pennsylvania State University, USA

Electrochemical supercapacitive devices, such as electric double layer capacitors and pseudocapacitors, are known for their high power density and long cycle life. In these devices, charges are stored at the interface between the electrode material and the electrolyte, giving rise to electrostatic double layer contributions and pseudocapacitive contributions to the total capacitance of the system. Among existing pseudocapacitive electrode materials, RuO_2 has been shown to exhibit a remarkably large pseudocapacitance; however, RuO_2 is too expensive for the mass production of pseudocapacitors. Therefore, considerable efforts have been devoted to developing cheaper electrode materials. In this research, we have carried out grand canonical Monte Carlo simulations based on the results of first principles calculations taking into account solvent effects within the electrolyte in order to clarify the charge storage mechanisms in pseudocapacitive electrode materials. Importantly, we have elucidated the sequence of adsorption reactions that take place on β - MnO_2 stoichiometric (110) surfaces upon raising the applied voltage. This comprehensive computational method enables us to predict key electrochemical properties of pseudocapacitor design to help guide their design and optimization.

S7: In situ Experiments of Microstructure Evolution and Properties

In Situ Experiments on Microstructural Evolution and Properties II

Room: Mediterranean A/B

Session Chairs: Shen Dillon, University of Illinois at Urbana-Champaign; Wayne Kaplan, Technion - Israel Institute of Technology

2:00 PM

(EMA-S7-004-2017) Atomic Scale In Situ Electron Microscopy: Challenges and Opportunities (Invited)

J. R. Jinschek^{*1}; 1. Thermo Fisher Scientific, Netherlands

Research on functional nanomaterials demands studies of structure, properties, and function, down to the atomic scale. To our advantage, atomic scale electron microscopy (EM) has become a powerful and indispensable tool for characterizing those nanostructures. Ongoing activities concentrate on methodological aspects of state-of-the-art EM and thereby open routes towards atom sensitive imaging of nanostructures that play a crucial role in numerous applications. However, the actual state and function of nanomaterials 'in operation' cannot always be inferred from examination under standard EM conditions or from postmortem EM studies. In-situ techniques enable visualization of structural evolution under operational conditions, thereby providing new insights in important materials science questions. EM imaging schemes will be discussed that focus on maintaining spatial resolution in in-situ studies, while controlling electron beam / structure interactions. Further development in in-situ EM stages will be highlighted as well. MEMS-based heating holder enable faster settling time with a more accurate knowledge of experimental conditions. Moreover, the integration into a gas-flow nanoreactor enables operando EM combining structural characterization. These advancements open up for unprecedented control over experimental conditions in advanced EM experiments of dynamic phenomena in materials sciences.

2:30 PM

(EMA-S7-005-2017) In-situ Transmission Electron Microscopy Observation of Heat-Induced Structural Changes of 3D Nb₃O₇(OH) Networks (Invited)

S. Betzler²; C. Scheu^{*1}; 1. Max-Planck-Institut für Eisenforschung GmbH, Germany; 2. Ludwig-Maximilians-University, Germany

Hydrothermally grown 3D networks consisting of Nb₃O₇(OH) nanowires are attractive candidates for solar-driven hydrogen production and solar cells. This is due to their high-surface area combined with suitable optical and electrical properties. The hydrothermal growth leads to crystalline nanowires (diameter ~ 40 nm) with a large number of stacking faults in their interior. The structural and morphological stability of the 3D networks is investigated with respect to temperature both ex-situ in air and in-situ under reducing atmosphere in the transmission electron microscopy (TEM). The in-situ TEM studies reveal the release of water from the crystal structure and the formation of an oxygen-deficient niobium oxide phase. At 450°C dislocations form at the nanowire interior defective region which move with a speed of around 5.9 ± 1.3 nm/min towards the surface. This initiates the phase transformation which is completed at temperatures above 750°C. To compensate the volume differences of the original orthorhombic Nb₃O₇(OH) crystal structure and the oxygen-deficient niobium oxide phase pores are formed. The in-situ TEM experiments also reveal an extremely high thermal stability of the morphology of the nanowire network, which is also confirmed by ex-situ heating investigations. The 3D morphology remains unchanged up to 850°C where merging of nanowires occurs.

3:00 PM

(EMA-S7-006-2017) Towards probing the barrier strength of grain boundaries for dislocation transmission (Invited)

G. Dehm^{*1}; N. Malyar¹; C. Kirchlechner¹; 1. Max Planck Institut für Eisenforschung, Germany

Grain boundaries are known to frequently act as barriers for dislocations in metals and thus usually enhance their strengths. Several models have been proposed which explain under which conditions dislocations are expected to pile-up at a grain boundary or to become transmitted into the neighboring grain. Miniaturized mechanical testing methods coupled with in situ electron microscopy and/or synchrotron techniques provide new possibilities to determine the barrier strength for dislocation transmission. In this talk we report on recent results concerning grain boundaries in Cu with a focus on coherent twin boundaries.

4:00 PM

(EMA-S7-007-2017) High-speed observation of the agglomeration of thin metal films on ceramic substrates (Invited)

K. van Benthem^{*1}; S. Hihath¹; M. Santala²; G. Campbell²; 1. University of California, Davis, USA; 2. Lawrence Livermore National Laboratory, USA

The agglomeration of thin films on ceramic substrates can occur in either the solid or liquid state for which different mass transport mechanisms are expected to control morphological changes. Traditionally, dewetting dynamics have been examined on time scales between several seconds to hours, and length scales ranging between nanometers and millimeters. In this study we have used dynamic transmission electron microscopy (DTEM) to directly observe the agglomeration of thin Ni films supported by SiO₂ and SrTiO₃ substrates. DTEM imaging was used to directly observe agglomeration kinetics, and confirmed that the initial stages of film agglomeration include edge retraction, hole formation and growth. Finite element modeling was used to simulate temperature distributions within the DTEM samples after laser irradiation with different energies. When the metal film reaches its melting point, ablation of nanometric droplets was observed while Marangoni flow dominates hole formation. In the solid state nucleation of voids occurs, as expected, mostly through surface diffusion. This work was financially supported by the US National Science Foundation through a NSF Faculty Early Career Award (DMR-0955638), and a UC Laboratory Fee grant (#12-LR-238313). Experiments at LLNL were carried out under the auspices of the US Department of Energy, Office of Basic Energy Sciences under contract DE-AC52-07NA27344.

4:30 PM

(EMA-S7-008-2017) In situ X-ray Photoelectron and Auger Electron Spectroscopic Characterization of Reaction Mechanisms during Li-ion Cycling of CuO Electrodes

C. Tang^{*1}; R. Haasch²; S. Dillon¹; 1. University of Illinois at Urbana-Champaign, USA; 2. Frederick Seitz Materials Research Laboratory, USA

Conversion behavior of metal oxides has proved to be a promising concept for Li-ion batteries. To this effect, there has been a significant amount of research devoted to understanding conversion reactions. Due to the sensitivity of electrodes to environmental exposure, in situ techniques are critical for understanding the complexity of reaction mechanisms. In this work we demonstrate, for the first time, in situ XPS and in situ AES combined with in situ SEM applied to characterizing the evolution of structure, bonding, and chemistry in CuO nanoparticle during cycling. We developed an open cell utilizing a Li permeable carbon membrane and ionic liquid. The membrane is able to isolate the nanoparticles from the electrolyte while simultaneously serving as a current collector. The electrolyte and counter electrode are sealed below the membrane. This cell provides good electrochemical control, while suppressing the solid electrolyte interface that could obscure underlying reactions of particles. We applied this method to study the insertion and extraction of Li from CuO nanoparticles during cycling. While XPS provided

important bonding information, AES was able to characterize the composition of individual particle agglomerates. These results provide new insights into irreversible reactions and side reactions that occur in CuO during cycling.

4:45 PM

(EMA-S7-009-2017) Nanoscale Atomic Displacements Ordering for Enhanced Piezoelectric Properties in Lead-Free ABO₃ Ferroelectrics

A. Pramanick^{*1}; 1. City University of Hong Kong, Hong Kong

The tuning of internal disorder in crystal lattices is often used as a means to influence mechanical, electrical, and thermal properties of materials. In many of the lead-free ferroelectric oxides, the local atomic displacements from high-symmetry lattice positions are correlated over only nanometer lengthscales, while the bulk electrical polarization emerges as an ensemble average over a given material volume. In this talk, I will present results from in situ x-ray diffuse scattering and inelastic neutron scattering experiments, which show how electric-field-induced ordering of local atomic displacements in lattices of prototype lead-free ABO₃ ferroelectrics can lead to enhanced electromechanical properties. The central mechanism for enhanced piezoelectricity is found to be an electric-field-induced nanoscale ordering of B atom displacements, which induces increased lattice instability and therefore a greater susceptibility for mechanical deformation. In general, a strong correlation between nanoscale ordering of atomic displacements and lattice instability suggest novel ways to enhance functional properties in lead-free ferroelectrics. References: A. Pramanick et al., *Advanced Materials* 27, 4330-4335, (2015) A. Pramanick et al., *Physical Review B: Rapid Communications* 88, 180101 (2013)

S10: Interfacial Phenomena in Multifunctional Heterostructures: From Theory to Transport Processes

Physical Properties of Quantum Confined Structures

Room: Caribbean B

Session Chairs: Jayakanth Ravichandran, Columbia University; Bharat Jalan, University of Minnesota

2:00 PM

(EMA-S10-022-2017) High Electron Mobility in Oxide Interfaces (Invited)

N. Pryds^{*1}; D. Christensen¹; G. Prawiroatmodjo²; F. Trier¹; M. von Soosten¹; Y. Zhang¹; T. Jespersen²; Y. Chen¹; 1. Technical University of Denmark, Denmark; 2. Niels Bohr Institute, University of Copenhagen, Denmark

One of the major and long-standing challenges of oxide 2DEGs is still to understand how to enhance the electron mobility. The mobility is still orders of magnitude lower than that of the conventional semiconductors and with the current fabrication method we still cannot fully control the charge at the interface. Here, I will present the recent activities of our group in this area where we try to push the mobility to record high values, i.e. the usage of the so-called modulation-doping technique has significantly increased the carrier mobility to mobility of 70,000 cm²/Vs and realization of quantum Hall effect in these films. These findings pave the way for studies of mesoscopic physics with complex oxides and design of high-mobility all-oxide electronic devices.

2:30 PM

(EMA-S10-023-2017) Electroforming of oxygen vacancies in SrTiO₃ evidenced by graphene quantum conductance (Invited)

W. Choi^{*1}; 1. SungKyunKwan University, Republic of Korea

Combination of functional properties in complex oxides and quantum transport behavior in graphene let us explore novel

physical phenomena and possible opto-electronic device applications. In this presentation, we will present examples of synergetic behavior in monolayer graphene on SrTiO₃ (STO) epitaxial thin film, using electrical transport measurements. First, we show that a large gate-voltage scaling in graphene transport is possible using STO. The graphene on epitaxial STO thin film shows quantum Hall state which survives up to 200 K at a magnetic field of 14 T. In addition, the substantial shift of charge neutrality point in graphene seems to correlate with the temperature-dependent dielectric constant of the STO thin film, and its effective dielectric properties could be deduced from the universality of quantum phenomena in graphene. [1] Second, using the quantum conductance, we probe the creation and annihilation of oxygen vacancies at graphene/STO surface. Since monolayer graphene is highly sensitive to the surrounding electronic environment without modifying it, we can exclusively understand the electronic reconstruction occurring in the STO layer due to oxygen vacancy formation. By analyzing the hysteretic current-voltage loops, we can quantitatively estimate the relation between the thickness, dielectric constant, and oxygen vacancy concentration in oxygen deficient STO layer.

3:00 PM

(EMA-S10-024-2017) Quantum Hall Effect in Bi/Sb Based Chalcogenide Topological Insulators (Invited)

V. V. Deshpande^{*1}; 1. University of Utah, USA

The half-integer quantum Hall (QH) effect of Dirac fermions has been a fertile area of research in graphene and has led to several interesting observations such as broken-symmetry QH states and fractional QH states. Topological insulators (TIs) such as Bi/Sb based chalcogenides are another Dirac system of great interest for spintronics and quantum computing applications. However, transport measurements have been plagued by problems of bulk conduction. Recently, three groups have overcome the bulk conduction problem and have observed the half-integer QH effect of Dirac fermions on the surface on these materials at very high magnetic fields. At the University of Utah, we have developed high quality single crystal synthesis of some of these materials. We observe the quantum Hall effect in the quaternary TI BiSbTeSe₂ at lower fields than previous groups. We are also exploring the use of boron nitride (BN) as a substrate for TIs. I will report on the energy gap of these QH states and also our latest results on TI/BN heterostructures.

4:00 PM

(EMA-S10-025-2017) Atomically engineered ferroic layers yield a room-temperature magnetoelectric multiferroic (Invited)

J. Mundy^{*1}; 1. University of California, Berkeley, USA

Materials that exhibit simultaneous order in their electric and magnetic ground states hold promise for use in next-generation memory devices in which electric fields control magnetism. Here we present a methodology for constructing single-phase multiferroic materials in which ferroelectricity and strong magnetic ordering are coupled near room temperature. Starting with hexagonal LuFeO₃—the geometric ferroelectric with the greatest known planar rumpling—we introduce individual monolayers of FeO during growth to construct formula-unit-thick syntactic layers of ferrimagnetic LuFe₂O₄ within the LuFeO₃ matrix, that is, (LuFeO₃)_m/(LuFe₂O₄)_n superlattices. The severe rumpling imposed by the neighbouring LuFeO₃ drives the ferrimagnetic LuFe₂O₄ into a simultaneously ferroelectric state, while also reducing the LuFe₂O₄ spin frustration. This increases the magnetic transition temperature substantially—from 240 K for LuFe₂O₄ to 281 K for (LuFeO₃)₉/(LuFe₂O₄)₁. Moreover, the ferroelectric order couples to the ferrimagnetism, enabling direct electric-field control of magnetism at 200 kelvin. Our results demonstrate a design methodology for creating higher-temperature magnetoelectric multiferroics by exploiting a combination of geometric frustration, lattice distortions and epitaxial engineering.

4:30 PM

(EMA-S10-026-2017) Disentangling growth induced and equilibrium properties of 2DEGs at oxide interfaces (Invited)

R. Dittmann^{*1}; C. Xu¹; R. Heinen¹; S. Hoffmann-Eifert¹; F. Gunkel²;
1. Forschungszentrum Juelich, Germany; 2. IWE II, RWTH Aachen University, Germany

2-dimensional electron gases (2DEGs) at oxide interfaces have attracted a significant amount of attention in recent years. Next to the charge accumulation induced by the polar character of the interfaces, the interface transport is strongly modified by the inherent defect concentrations present in thermodynamic equilibrium as well as by additional defects induced by non-equilibrium growth conditions. In order to discriminate non-equilibrium interface properties from the equilibrium state, we perform high temperature equilibrium conductance measurements of different types of oxide interfaces and investigate the impact of growth and annealing conditions. For different epitaxial heterostructures grown at high temperature, we find an equilibrium state which is independent on the growth pressure and can be attributed to the formation of a thermodynamically stable space charge layer (SCL), in which electrons as well as ionic cation vacancies accumulate. We conclude that the SCL is stabilized by the electrostatic boundary conditions derived from the polar catastrophe. For initially amorphous LAO/STO grown at room temperature, the equilibrium conductance is found to be identical to the one of bare STO. This system thus relies on a thermodynamic non-equilibrium state based on the formation of oxygen vacancies during growth, which vanish in thermodynamic equilibrium.

S11: Ion Conducting Ceramics**Design and Characterization of Ion Conducting Ceramics**

Room: Caribbean C

Session Chair: Jon Ihlefeld, Sandia National Laboratories

2:00 PM

(EMA-S11-007-2017) Accelerated Design and Discovery of Fast Ion Conducting Materials using First Principles Computation (Invited)

Y. Mo^{*1}; 1. University of Maryland, College Park, USA

The design and discovery of new ionic materials have been pursued through a trial-and-error manner, which is time consuming and labor intensive. First principles computation, which can predict materials properties with little experimental input, has the potential to accelerate the development of new ionic conductor materials. In this presentation, I will demonstrate the state-of-the-art first principles computation methods to design and discover ion conductor materials for all-solid-state Li-ion batteries, solid oxide fuel cells, and hydrogen separation. I will first show the use of first principles computation to provide unique materials insights, such as in determining the origin of fast ionic diffusion and identifying the key limiting factors in these ion conductors. The first principles computation methods in predicting the phase stability, chemical/electrochemical stability, ionic diffusional properties, and polaron formation as a function of experimental conditions will be demonstrated to design new materials. Multiple new materials with enhanced properties will be designed using the accelerated first principles approach, and will be confirmed in multiple experimental studies. Our first principle calculation demonstrates the new direction of accelerated computation design and discovery for high-performance ionic conductor materials.

2:30 PM

(EMA-S11-008-2017) Fast Atomic-Scale Chemical Imaging by Scanning Transmission Electron Microscopy for Study of Dynamic Phase Transformations (Invited)

P. Lu^{*1}; R. Yuan²; J. Ihlefeld¹; E. D. Spörke¹; J. Zuo²; W. Pan¹; 1. Sandia National Laboratories, USA; 2. University of Illinois at Urbana-Champaign, USA

Ability to study phase transformation at atomic-scale and particularly follow structural change at different stages of the phase transformation is critical to materials research. Scanning transmission electron microscopy (STEM) using energy-dispersive x-ray spectroscopy (EDS) offers the capability of chemical imaging at atomic-scale. Recently we have shown rapid atomic-scale chemical imaging can be achieved by using a lattice-vector translation method. The technique provides atomic-scale chemical maps averaged over an area of \sim few 10 nm² acquired with the acquisition time of \sim 2 s or less, allowing for investigation of dynamic material phenomena. In this talk we report details of the method, and particularly investigate the conditions for achieving the fast chemical mapping. As the first example of its application, the technique is applied to study phase transformation in beam-sensitive Li[Li_{0.2}Ni_{0.2}Mn_{0.6}]O₂ (LNMO) lithium ion battery cathode material. The application of this technique for study of ion conducting materials will also be explored. *Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:00 PM

(EMA-S11-009-2017) The Effect of Non-stoichiometry and Lattice Strain on the Proton Conductivity in Y-Doped Barium Zirconate

J. Ding²; X. Sang¹; J. Balachandran¹; W. Guo¹; C. Rouleau¹; G. Veith¹; C. Bridges¹; J. Poplawsky¹; N. Bassiri-Gharb²; P. Ganesh^{*1}; R. Unocic¹;
1. Oak Ridge National Lab, USA; 2. Georgia Institute of Technology, USA

Yttrium doped barium zirconate (Y-BZO) has been widely studied as a promising electrolyte for proton-conducting solid oxide fuel cells, due to its high proton conductivity and excellent chemical stability at intermediate temperatures. While crucial to the ionic conductivity, the fundamental role of non-stoichiometry and extended defects in Y-BZO has not been well understood. In this study, (100) oriented 20% Y doped BZO single crystal thin films were prepared by pulsed layer deposition. For comparison, sample with lattice strain was induced by varying substrates, and the non-stoichiometry was induced by annealing at 1000°C for 24 h. Their effects on atomic resolution structure and the activation barrier for proton conduction were quantified by a combined suite of characterization techniques. We found that barium deficient regions formed after annealing, resulting lower total proton conductivity, contrary to a recent claim that Ba deficient compositions show superior conductivity. In addition, compressive strain was detrimental to proton conductivity due to confined pathways for proton hopping. We also explored the idea of in-situ phase transformation by electron beam, where Ba-deficient region transforms to a more ordered, defect-free phase after beam exposure. This might be a novel approach to remove non-stoichiometry locally and improve the overall conductivity.

3:15 PM

(EMA-S11-010-2017) Improved Ionic Conductivity in Doped Ceria by Sintering in Reducing Atmosphere

S. Sulekar^{*1}; J. Kim¹; J. C. Nino¹; 1. University of Florida, USA

Rare earth doped ceria is greatly suited for use as an electrolyte for intermediate temperature solid oxide fuel cells. When doped with trivalent acceptor dopants, oxygen vacancies are generated which act as charge carriers leading to ionic conductivity. During sintering, the dopants tend to segregate to the grain boundaries in ceria. Atom

probe tomography in Nd doped ceria has shown that Nd ions and oxygen vacancies segregate at grain boundaries, with the compositional difference extending up to 5-6 nm from the structural center of the grain boundary.¹ This high concentration of dopants and defect-defect interaction at the grain boundaries makes them highly resistive and causes a drop in the overall ionic conductivity and performance. Various techniques like fast firing and microwave sintering have been used to reduce this dopant segregation issue. Here we try a different approach, where doped ceria is sintered under a reducing atmosphere using 4% H₂-N₂ at lower temperatures as compared to conventional sintering. The reducing atmosphere is hypothesized to change the valence of cerium ions from Ce⁺⁴ to Ce⁺³ (similar to the dopant ions e.g. Gd⁺³), thus reducing the tendency for preferential segregation of the dopant. The ionic conductivity of the doped ceria samples thus obtained will be discussed. References: 1. Diercks, D. R. et al. J Mater Chem A 4, 5167–5175 (2016).

4:00 PM

(EMA-S11-011-2017) Enhancing Grain Boundary Ionic Conductivity in Mixed Ionic–Electronic Conductors

F. Chen^{*1}; 1. University of South Carolina, USA

Mixed ionic-electronic conductors are widely used in devices for energy conversion and storage. Grain boundaries in these materials have nanoscale spatial dimensions, which can generate substantial resistance to ionic transport due to dopant segregation. Here we report the concept of targeted phase formation in a Ce_{0.8}Gd_{0.2}O_{2-δ}-CoFe₂O₄ composite that serves to enhance the grain boundary ionic conductivity. Using spatially resolved electron microscopy and spectroscopy, we probe the grain boundary charge distribution and chemical environments altered by the phase reaction between the two constituents. The formation of an emergent phase successfully avoids segregation of the Gd dopant and depletion of oxygen vacancies at the Ce_{0.8}Gd_{0.2}O_{2-δ}-Ce_{0.8}Gd_{0.2}O_{2-δ} grain boundary. This results in superior grain boundary ionic conductivity as demonstrated by the enhanced oxygen permeation flux. This work illustrates the control of mesoscale level transport properties in mixed ionic-electronic conductor composites through processing induced modifications of the grain boundary defect distribution

4:15 PM

(EMA-S11-012-2017) Amphoteric Transition Metal Ions: New Insights into Novel Perovskite Doping Mechanisms

R. A. Maier^{*1}; A. Johnston-Peck¹; M. Donohue²; 1. National Institute of Standards and Technology, USA; 2. National Institute of Standards and Technology, USA

For the common perovskite chemistries like SrTiO₃, the recipe has always been straight-forward and simple. Introduce a transition metal ion impurity to the lattice, and it will more often than not sit on the B-site and act as an acceptor. For the first time, direct evidence will be provided that manganese does not obey this general rule. Electron paramagnetic resonance and high-resolution transmission electron microscopy methods were employed to determine the site occupancy and charge compensation mechanisms of manganese ions in the SrTiO₃ lattice. It will be demonstrated that manganese acts as an amphoteric dopant in stoichiometric SrTiO₃ with Mn⁴⁺ placed on the B-site and Mn²⁺ placed on the A-site at a roughly 1:1 ratio. If the Sr/Ti stoichiometry is tuned, the site occupancy of manganese can be adjusted. The resulting oxygen vacancy concentration is shown to be controlled mostly by the Sr/Ti stoichiometry rather than the manganese contribution with Sr-rich inter-planar growth (or Ruddlesden-Popper phases) acting as potential oxygen vacancy sinks. Implications on dielectric reliability and insight into transition metal amphoteric doping in comparable perovskite systems will be discussed.

S15: Superconducting Materials and Applications

Applications and Related Material Issues including Wire Properties

Room: Pacific

Session Chairs: Alex Gurevich, Old Dominion University; Arend Nijhuis, University of Twente

2:00 PM

(EMA-S15-033-2017) Status of Cryogenic/Superconducting Power System Technologies for Electrified Propulsion of Aircraft (Invited)

T. J. Haugan^{*1}; 1. U.S. Air Force Research Laboratory, USA

Hybrid-electric-vehicle (HEV) or electric-vehicle (EV) propulsion is well understood from the automotive industry, and achieves very significant increases of energy efficiencies of 2-3x from the use of non-combustion technologies and 'smart' energy management including brake regeneration. The use of battery-electric and hybrid-electric propulsion for aircraft has increasingly been realized in the last 5 years, and has been successfully implemented in 2 and 4 passenger aircraft. In 2016, it's expected that certification of electric propulsion will be achieved for small aircraft. This paper will summarize recent progress of this field for aircraft, and present case studies of how cryogenic/superconducting electric power systems can positively impact hybrid-electric or all-electric power systems and capabilities, for different size and power level aircraft. Cryogenic drivetrain and components studied include generators and motors, power transmission cables, power storage devices including Li-batteries and superconducting magnetic energy storage (SMES), power electronics including inverters, and cryocooling technologies. Properties of cryogenic systems and components will be presented, including technical readiness level and scaling of power densities for varying power level, and these properties will be compared to Cu-wire based systems.

2:30 PM

(EMA-S15-034-2017) Modelling and Testing of MgB₂ Segmented Coils and Persistent joints for MgB₂ Magnets (Invited)

M. Sumption^{*1}; 1. The Ohio State University, USA

This study focusses on a few technology areas needed to enable 3 T R&W whole body conduction-cooled MgB₂-based MRI development. We have developed magnetic designs for a 3 T MgB₂ MRI system optimized for minimizing conductor length at 4 K operation, but with conduction cooling. The tradeoffs for different conductor designs are presented, and also the design constraints at different maximal thermal gradients along the coil. We also present initial studies on mechanical thermal design, integrated with the magnet design. Experimentally, an MgB₂ coil segment was also tested at 10 K in self field for I_c. The coil was cooled by conduction cooling and magnetic fields, strains, and temperature gradients were measured. The coil was well instrumented, and had heaters which we used for the study of quench propagation and quench protection. The response of the system to various disturbances was explored, and two regimes of protection are described. Quench propagation and protection are seen to have somewhat different characteristics for MgB₂ than for conventional LTS systems. We also present the results of persistent joint development. A persistent current was induced in a small coil and its decay measured. These measurements were performed at 4.2 K, in fields up to 7 T. Joint resistances of 10⁻¹² ohms were observed, and with I_c values of 300 A at zero field and 200 A at 3 T.

3:00 PM**(EMA-S15-035-2017) The MgB₂ superconductor: A case study of the relationship between basic science research to superconducting applications (Invited)**

M. A. Susner^{*2}; M. Sumption³; G. Li³; S. Bohnenstiehl³; Y. Yang³;
T. J. Haugan¹; E. W. Collings³; 1. U.S. Air Force Research Laboratory, USA;
2. UES, Inc., USA; 3. Ohio State University, USA

The phenomenon of superconductivity is one of the most exciting, and sometimes frustrating, areas of condensed matter physics research. From a basic science perspective, most discoveries of superconducting materials have either been serendipitous or have relied on chemical intuition based off of already known superconducting materials. From an applied science perspective, the engineering and commercialization of superconducting materials requires the tailoring of electrical, materials, and mechanical engineering to the material in question to optimize superconductive properties such as critical current density, upper critical field, flux pinning density, and transition temperature. In this talk I shall discuss the collaborative efforts of The Ohio State University, Hyper-Tech Research, Inc., and the Air Force research Laboratory to study the fundamental properties of MgB₂, the alteration of these properties based on intrinsic or extrinsic effects such as doping or grain size, and the application of these lessons to the development of superconducting wires for commercial applications such as MRI magnets or wind turbines.

3:30 PM**(EMA-S15-036-2017) Understanding High Temperature Superconductors for Potential use in Aero-Engine components**

D. E. Sievers^{*1}; 1. The Boeing Co., USA

High temperature superconductivity is a broad subject and contains numerous materials and compounds for potential discussion. This paper will focus on one (1) type of superconductor; Bulk (RE) YBaCuO. Rare earths (RE) have been found to increase superconductivity aspects of YBaCuO bulk systems when replacing Yttria with a rare earths such as Nd, Eu, Gd, Er, La. Superconductivity was realized in the early 20th century by Kamerlingh-Onnes through utilizing liquid helium to cool various metals to 4.2 Kelvin and over the years has advanced into obtaining levitation at higher temperatures, such as the Maglev train in Japan, with hundreds of alloys and compounds opening the realm of technology into many industries. High temperature bulk superconductors, 77K, allows them to be more manageable for practical applications such as high speed rail, frictionless bearings, and electric motors. This paper will focus specifically on the state of the art of processing, structure, properties, and performance of bulk (RE)YBaCuO superconductors and their application in hybrid electric aircraft.

3:45 PM**(EMA-S15-006-2017) Development and control of physical properties of new layered compounds with CrPn layers**

Y. Ichihara^{*1}; H. Ogino²; J. Shimoyama³; K. Kishio¹; 1. University of Tokyo, Japan; 2. National Institute of Advanced Industrial Science and Technology (AIST), Japan; 3. Aoyama Gakuin Univ., Japan

Fe-based superconductors reported by Hosono et al. in 2008 have attracted great attention because of its relatively high T_c. These structures consist of alternating stack of antiferromagnetic type FePn (Pn = As, P) layer and blocking layer such as an oxide layer. In addition, superconductors with NiPn layers are reported, and they contain TM cation with even number of d electrons. In this study materials contain CrPn layer are focused because they also have even number of d electrons and binary compound CrAs shows superconductivity, therefore a new superconductor with CrPn layer is expected. Based on these facts, synthesis of new layered compounds with CrPn layer and control of physical properties of these compounds have been attempted to discover a new superconductor. All samples were prepared by the solid state reaction. Resistivity and magnetic susceptibility of new compounds were measured by PPMS and

MPMS. As a result, 11 new compounds such as (Cr₂Pn₂)(Sr₄Sc₂O₆) (Pn = As, P) and BaCr₂P₂ have been discovered. There are correlation between a-axis length and physical properties of new compounds, for example compounds with shorter a-axis length show lower resistivity. In this study, control of physical properties of (Cr₂As₂)(Sr₄Sc₂O₆) and BaCr₂P₂, which have short a-axis length among new compounds, was tried by chemical substitution.

S16: Failure: The Greatest Teacher**Failure: The Greatest Teacher**

Room: Indian

Session Chair: Geoff Brennecke, Colorado School of Mines

5:35 PM**(EMA-S16-003-2017) Intuition vs. Thermodynamics (or Maybe We Should Have Calculated That First!)**

M. Losego^{*1}; 1. Georgia Institute of Technology, USA

Sometimes an experiment surprises you. But should it have? Maybe it would have been better to do a few calculations first. (Ah, but what experimentalist wants to do that?) In this talk a few examples will be given of when a calculation may have been a good idea prior to an experiment. (Likely ~5 min, certainly less than 10 min)

5:45 PM**(EMA-S16-004-2017) The First FRAM - Extraordinary Success, Painful Failure**

J. T. Evans^{*1}; 1. Radiant Technologies, Inc., USA

Krysalis Corporation designed and built the first fully functional CMOS FRAM in 1987 in Albuquerque, NM. The first die on the first wafer of the first lot was fully functional. Despite this miracle, Krysalis failed. Hear one of the founders tell this story and his lessons learned.

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