

The American Ceramic Society
2020 Conference on Electronic Materials
and Applications (EMA 2020)

ABSTRACT BOOK

January 22–24, 2020
Orlando, Florida

Introduction

This volume contains abstracts for 333 presentations during the 2020 Conference on Electronic Materials and Applications (EMA 2020) in Orlando, Florida. The abstracts are reproduced as submitted by authors, a format that provides for longer, more detailed descriptions of papers. The American Ceramic Society accepts no responsibility for the content or quality of the abstract content. Abstracts are arranged by day, then by symposium and session title. An Author Index appears at the back of this book. The Meeting Guide contains locations of sessions with times, titles and authors of papers, but not presentation abstracts.

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.

Copyright © 2020 The American Ceramic Society (www.ceramics.org). All rights reserved.

MEETING REGULATIONS

The American Ceramic Society is a nonprofit scientific organization that facilitates the exchange of knowledge meetings and publication of papers for future reference. The Society owns and retains full right to control its publications and its meetings. The Society has an obligation to protect its members and meetings from intrusion by others who may wish to use the meetings for their own private promotion purpose. Literature found not to be in agreement with the Society's goals, in competition with Society services or of an offensive nature will not be displayed anywhere in the vicinity of the meeting. Promotional literature of any kind may not be displayed without the Society's permission and unless the Society provides tables for this purpose. Literature not conforming to this policy or displayed in other than designated areas will be disposed. The Society will not permit unauthorized scheduling of activities during its meeting by any person or group when those activities are conducted at its meeting place in interference with its programs and scheduled activities. The Society does not object to appropriate activities by others during its meetings if it is consulted with regard to time, place, and suitability. Any person or group wishing to conduct any activity at the time and location of the Society meeting must obtain permission from the Executive Director or Director of Meetings, giving full details regarding desired time, place and nature of activity.

Diversity Statement: The American Ceramic Society values diverse and inclusive participation within the field of ceramic science and engineering. ACerS strives to promote involvement and access to leadership opportunity regardless of race, ethnicity, gender, religion, age, sexual orientation, nationality, disability, appearance, geographic location, career path or academic level.

Visit the registration desk if you need access to a nursing mother's room or need further assistance. For childcare services, please check with the concierge at individual hotels for a listing of licensed and bonded child care options.

The American Ceramic Society plans to take photographs and video at the conference and reproduce them in educational, news or promotional materials,

whether in print, electronic or other media, including The American Ceramic Society's website. By participating in the conference, you grant The American Ceramic Society the right to use your name and photograph for such purposes. All postings become the property of The American Ceramic Society.

During oral sessions conducted during Society meetings, **unauthorized photography, videotaping and audio recording is prohibited**. Failure to comply may result in the removal of the offender from the session or from the remainder of the meeting.

Registration Requirements: Attendance at any meeting of the Society shall be limited to duly registered persons.

Disclaimer: Statements of fact and opinion are the responsibility of the authors alone and do not imply an opinion on the part of the officers, staff or members of The American Ceramic Society. The American Ceramic Society assumes no responsibility for the statements and opinions advanced by the contributors to its publications or by the speakers at its programs; nor does The American Ceramic Society assume any liability for losses or injuries suffered by attendees at its meetings. Registered names and trademarks, etc. used in its publications, even without specific indications thereof, are not to be considered unprotected by the law. Mention of trade names of commercial products does not constitute endorsement or recommendations for use by the publishers, editors or authors.

Final determination of the suitability of any information, procedure or products for use contemplated by any user, and the manner of that use, is the sole responsibility of the user. Expert advice should be obtained at all times when implementation is being considered, particularly where hazardous materials or processes are encountered.

Copyright © 2020. The American Ceramic Society (www.ceramics.org). All rights reserved.

Table of Contents

Wednesday, January 22, 2020

Plenary Session I	7
S1: Characterization of Structure–Property Relationships in Functional Ceramics	
Probing Structure Property Correlations in Ceramics	7
Advanced Electron Microscopy Methods for Characterization of Functional Ceramics	8
S2: Advanced Electronic Materials: Processing Structures, Properties, and Applications	
Applications of Advanced Electronic Materials	10
Electromechanical Properties and Structure of Bulk and Film Electronic Materials	11
S3: Frontiers in Ferroic Oxides: Synthesis, Structure, Properties, and Applications	
Ferroelectric and Dielectric Oxides	13
Magnetism, Structure, and Defects in Transition Metal Oxides	14
S4: Complex Oxide Thin Film Materials Discovery: From Synthesis to Strain/Interface Engineered Emergent Properties	
Enhanced Functionality through Advanced Synthesis	16
Advanced Complex Oxide Thin Film Synthesis I	17
Advanced Synthesis II	18
S8: Structure–Property Relationships in Relaxor Ceramics	
Local Structure of Relaxors I	20
Local Structure of Relaxors II	22
Perovskite/Non-perovskite Relaxors I	22
S10: Point Defects and Transport in Ceramics	
Predictive Point Defect Energetics and Equilibria from Density Functional Theory and other Computational Methods	23
Structure and Mobility of Defects and Defect Complexes	25

S12: Electronic Materials Applications in 5G Telecommunications	
Industry and 5G	26
Theory, Modeling, and New Measurement Modalities in 5G.....	28
S14: Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics	
Materials by Design	29
Predictive Modeling/Novel Phenomena.....	31
Poster Session.....	33
Thursday, January 23, 2020	
Plenary Session II.....	40
S1: Characterization of Structure–Property Relationships in Functional Ceramics	
Probing Defects and Disorder in Functional Ceramics.....	40
S2: Advanced Electronic Materials: Processing Structures, Properties, and Applications	
Lead-free and Relaxor Ferroelectrics	41
Synthesis of Electronic Materials and the Role of Defects.....	42
S3: Frontiers in Ferroic Oxides: Synthesis, Structure, Properties, and Applications	
Ferroelectric Architectures and Devices	44
S4: Complex Oxide Thin Film Materials Discovery: From Synthesis to Strain/Interface Engineered Emergent Properties	
Engineered Interface Phenomena I	45
Engineered Interface Phenomena II.....	46
Machine Learning Driven Synthesis.....	47
S6: Complex Oxide and Chalcogenide Semiconductors: Research and Applications	
Design and Discovery of Complex-Structured Semiconductors	48

S7: Superconducting and Magnetic Materials: From Basic Science to Applications	
Superconducting and Magnetic Materials I.....	49
Superconducting and Magnetic Materials II.....	50
S8: Structure–Property Relationships in Relaxor Ceramics	
Perovskite/Non-perovskite Relaxors II.....	51
Novel Relaxors.....	52
Advanced Characterization of Relaxors.....	52
S9: Ion Conducting Ceramics	
Ion Conducting Ceramics for Solid-State Battery.....	53
S10: Point Defects and Transport in Ceramics	
Defect Mediated Properties (Conductivity, Grain Growth, Creep, Magnetism, Ferroelectric Imprint, Dielectric Degradation).....	55
S12: Electronic Materials Applications in 5G Telecommunications	
5G Measurement Science.....	56
Industry Panel and Tutorials.....	57
S13: Thermal Transport in Functional Materials and Devices	
Thermal Transport.....	58
S14: Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics	
High-throughput Approaches/Data Analytics I.....	59
High-throughput Approaches/Data Analytics II.....	60
Multiscale modeling.....	61
S16: Molecular, Inorganic, and Hybrid Ferroelectrics for Optoelectronic and Electronic Applications	
Metal-organic Halide Perovskites.....	62
Beyond Metal-organic Halide Perovskites.....	63

Friday, January 24, 2020

S4: Complex Oxide Thin Film Materials Discovery: From Synthesis to Strain/Interface Engineered Emergent Properties

Novel Synthesis Techniques 64

S5: Mesoscale Phenomena in Ferroic Nanostructures: Beyond the Thin-Film Paradigm

Modeling, Simulation and Processing 65

S6: Complex Oxide and Chalcogenide Semiconductors: Research and Applications

Low Dimensional Systems 67

Advanced Characterization of Physical and Chemical Properties 68

S7: Superconducting and Magnetic Materials: From Basic Science to Applications

2D Correlated Materials I 69

2D Correlated Materials II 70

Tailoring Properties of Superconducting and Magnetic Materials 71

Application of Superconducting Materials 71

S9: Ion Conducting Ceramics

Fundamental Processes and Characterizations in Ion Conducting Ceramics for Energy Storage 72

Emerging Ion Conducting Ceramics: Oxide and Halide 73

S11: New Directions in Sintering and Microstructure Control for Electronic Applications

New Directions in Sintering and Microstructure Control 73

S15: Functional Materials for Biological Applications

Synthesis, Functionalization, and Characterization of Biomaterials 76

Therapeutic, Diagnostic, and Biosensing Applications 77

Failure: The Greatest Teacher 78

Wednesday, January 22, 2020

Plenary Session I

Room: Orange A

Session Chair: Alp Schirlioglu, Case Western Reserve University

8:40 AM

(EMA-PLEN-001-2020) Novel Functionalities in Atomically Controlled Oxide Heterostructures by Pulsed Laser Deposition

G. Rijnders*¹

1. University of Twente, MESA+ Institute for Nanotechnology, Netherlands

Complex oxides of the transition metals are of great importance and interest both from a fundamental science as well as a technological point of view. With regards to fundamental science, complex oxides show an interplay between strong electron correlations, band behaviour, as well as rich repertoire of ordering phenomena in the spin and orbital sectors making them an enduring focus of theoretical and experimental investigation. Recent progress in epitaxy-based thin film growth approaches has added a dimension to complex oxide research, providing opportunities to improve experimental control over the properties of the system. We now possess a number of tools that can be used to design novel functionalities in complex oxides. We have demonstrated recently that strong oxygen octahedral coupling at interfaces transfers the octahedral rotation from one oxide into the other at the interface region. As a result, we possess control of magnetic and electronic properties by atomic scale design of the oxygen octahedral rotation. In this contribution I will highlight recent work on magnetic anisotropy in manganites, as well as the control of the metal-to-insulator transition temperature in nickelate heterostructures and superlattices.

S1: Characterization of Structure-Property Relationships in Functional Ceramics

Probing Structure Property Correlations in Ceramics

Room: Citrus B

Session Chair: Abhijit Pramanick, City University of Hong Kong

10:00 AM

(EMA-S1-001-2020) Influence of Adsorption on Equilibrium Metal-Ceramic Orientation Relationships (Invited)

H. Nahor¹; T. Mao¹; W. D. Kaplan*¹

1. Technion - Israel Institute of Technology, Department of Materials Science and Engineering, Israel

Metal-ceramic interfaces determine the mechanical and functional properties of many technologically important material systems, and thin metal films on ceramic substrates have an important role in technological applications and in fundamental science. Often, the orientation relationship (OR) of the polycrystalline metal film on the ceramic substrate influences the properties, and understanding why specific orientation relationships develop is thus important. While the details of metastable ORs depend on the kinetics of the specific deposition process, equilibrium (minimal energy) ORs define the driving force for microstructural evolution during annealing of thin films. As such, this study examines equilibrium ORs of metals on α -Al₂O₃ and yttrium stabilized zirconia (YSZ). Equilibrium conditions were reached by dewetting the thin films in the solid-state (annealing until the film ruptures and forms single crystal particles), and the influence of dopants and impurities on the equilibrium crystal shape of the metal, the low-energy OR of the metal with the substrate, and the interface energy, was assessed. This presentation will show that while specific low-index low-energy ORs often exist, adsorption to the same metal-ceramic interfaces can lower high-energy ORs, resulting in a more isotropic distribution at equilibrium.

10:30 AM

(EMA-S1-002-2020) Nanocomposite Electrolyte: New insights into Interactions between different oxide surfaces and a salt matrix above T_g (Invited)

M. A. Gulgun*¹; S. Shawuti¹; S. Mete¹; M. Sezen²; C. Ow-Yang¹

1. Sabanci University, FENS MatSE and NanoEng, Turkey
2. Sabanci University Nanotechnology Application Center, Turkey

Above T_g, an amorphous salt matrix with dispersed oxide nanoparticles in it behaves like a suspension, commonly known in ceramics industry as slurry. Impedance measurements of nanocomposite electrolytes with oxide nanoparticles of different surface charges revealed the influence of oxide Surface charges in dissociating the salt molecules in the amorphous matrix above T_g. The composite electrolyte appeared to have formed a supercooled structure similar to electrical double layer in ceramic particle suspensions. Nanocomposites consisting of an amorphous carbonate salt matrix and nanometer scale oxide particles are a possible candidate electrolyte for Intermediate Temperature range Fuel Cells. Several groups have claimed that the ionic transport in these hybrid electrolytes does not happen in solid oxide or the matrix phase but at the interface between them. The electrical double layer concept in supercooled liquids appear to support these claims. Experiments with carbonate salt matrices with dispersed nanoparticles in them with surface charges ranging from very acidic (pH ~2) to very basic (pH ~12) have shown that the interaction and hence ionic conductivity is tunable to some extent. We will elaborate on the oxide surface amorphous solid matrix interaction and some difficulties in the interpretation of impedance measurements in these composite ionic conductors.

11:00 AM

(EMA-S1-003-2020) Multiscale electro-mechanical response in ferroelectrics (Invited)

Y. Ivry*¹; M. Barzilay¹; H. Elangoval¹; A. Hershkovitz¹

1. Technion - Israel Institute of Technology, Israel

Being a sub-group of piezoelectric materials, ferroelectrics are widely used in electro-mechanical technologies, including ultrasound imaging and cellular communication. Hence, there is a strong motivation to understand and control the origin of the electro-mechanical activity in ferroelectrics. Traditional piezoresponse refers to a collective expansion or contraction of all unit cells together under external electric field. However, the electro-mechanical coupling in ferroelectrics is much richer and involves e.g. switching of individual elastic domains and bundles of elastic domains. Here we discuss the onset of electro-mechanical activity in the prototype perovskite ferroelectrics BaTiO₃. By comparing effects of electric field on the elastic properties to effects of temperature on these properties we reveal the multi-scale nature of the electro-mechanical coupling in ferroelectrics.

11:30 AM

(EMA-S1-004-2020) Anisotropy at Interfaces in Rare-Earth Pyrosilicates for High-Temperature Coatings and Halide Perovskites for Solar Cells

H. Sternlicht*¹; D. Huber²; D. W. McComb²; N. P. Padture¹

1. Brown University, School of Engineering, USA
2. The Ohio State University, USA

Anisotropy at interfaces has been shown long ago to affect microstructural evolution and properties of materials. This includes, and is not limited to, modified kinetics of reactions, as well as variation in the type of reactions, occurring at different interfaces. These will be discussed in two ceramic systems. Environmental barrier coatings (EBCs) are used to protect ceramic matrix composites (CMCs) used in the hot section of gas turbine engines against oxidation, and have to be resistant to attack of calcia-magnesia-alumino-silicate (CMAS) particles from the atmosphere, which can lead to premature

*Denotes Presenter

coatings failure. Electron microscopy characterization of the anisotropy in the CMAS- EBCs reaction will be discussed. In addition, degradation processes in halide perovskites (HPs) used for low cost and highly efficient solar cells, occurring at different interfaces will be demonstrated and discussed in light of the HPs sensitivity to the electron beam.

11:45 AM

(EMA-S1-005-2020) Time-Resolved Neutron Scattering Reveals Insight into Proton Motion in Organic Ferroelectric

C. Fancher^{*1}; A. Schultz²; C. Hoffmann¹; X. Wang¹

1. Oak Ridge National Lab, USA
2. Argonne National Lab, USA

Organic electronics are attractive due to their light-weight, low cost, flexibility and environmentally benign properties. Applications currently range from photoelectric cells to organic light emitting diodes (OLED) phones and TV screens, and to non-volatile ferroelectric memory. Organic ferroelectrics have been hypothesized to involve proton transfer when the polarization is switched, which can be characterized with only limited precision using X-ray tools. Recently we developed methods that enable time-resolved single crystal neutron diffraction at the Spallation Neutron Source at the Oak Ridge National Laboratory. In this paper, we present recent time-resolved diffraction results on the molecular ferroelectric material potassium dihydrogen phosphate (KDP). These results provide evidence that the electric field induced hydrogen bond redistribution is accompanied by a 90° lattice rotation. Single crystal structure analysis of electric field dependent diffraction data will be presented.

Advanced Electron Microscopy Methods for Characterization of Functional Ceramics

Room: Citrus B

Session Chairs: Chris Fancher, Oak Ridge National Lab; Hadas Sternlicht, Brown University

2:00 PM

(EMA-S1-006-2020) Hematite for light induced water splitting: Improving efficiency by tuning distribution of Sn dopants at the atomic scale (Invited)

S. Zhang¹; C. Scheu^{*1}

1. Max-Planck-Institut fuer Eisenforschung, Germany

Light induced water splitting is one way to convert solar energy and store them in hydrogen. This is important for a hydrogen economy to power cars and trucks by fuel cells. Hematite (α -Fe₂O₃) has been investigated for several decades as a photoanode material for water splitting. The absorption in the visible regime is excellent. However, the separation and the transfer of photogenerated charge carriers have low efficiencies, which can be improved by doping, e.g. with Sn. In our work we analyzed in depth the distribution of Sn in ultrathin Fe₂O₃ layers (thickness less than 20 nm) at the atomic scale by various transmission electron microscopy techniques combined with atom probe tomography. Submonolayer coverage of Sn at the surface passivated recombination sites, leading to more efficient hole transfer. When Sn was distributed over several atomic layers on the top, an additional boost in charge separation was achieved due to formation of a local electrical field. For higher amount of Sn, we were able to detect Sn segregation at the grain boundaries, which degrades the crystallinity of Fe₂O₃ and hence the overall performance. The authors would like to thank the colleagues and co-workers who contributed to this work and the German Research Foundation (DFG) for financial support within the Priority Programme SPP 1613.

2:30 PM

(EMA-S1-007-2020) Understanding the Structure of LiMn₂O₄ by Aberration-Corrected HAADF STEM and Differential Phase Contrast (Invited)

P. Ferreira^{*1}

1. IST/INL, Portugal and University of Texas, Austin, MSE, USA

The rising need for portable energy storage has led to the creation of a formidable Li-ion battery industry. Of the many cathode chemistries for Li-ion batteries, Li[Mn₂]O₄(LMO) stands out as an appealing cathode due to its moderate capacity, use of environmentally-friendly and cost-effective Mn, and high rate capabilities associated with its cubic spinel 3D framework. Yet, this material has shown capacity loss, due to the dissolution of Mn to the electrolyte. In this work we show by HAADF STEM that a restructured surface is formed in this material, where a stable surface layer of Mn₃O₄, followed by Li_{1+x}Mn₂O₄ subsurface is formed. In addition, recent advances in STEM allow us to obtain images proportional to the projected potential, projected electric field and projected charge distribution, by using differential phase contrast technique (DPC). Thus, we use DPC to determine the Li, Mn and O atomic positions, thus providing a novel insight into the structure of LiMn₂O₄. Our results show local regions depleted in Li and the existence of Mn atoms in tetrahedral sites occupying a typical Li atom position, or occupying a free octahedral site in the same column, in agreement with the Mn disproportionation reaction reported for such compound. These findings contribute to a better understanding of the mechanisms of lithium and manganese exchange in LiMn₂O₄ spinel structures.

3:00 PM

(EMA-S1-008-2020) Correlation between structure and chemistry at delithiated LiFePO₄ interface characterized by 4D-STEM and X-ray microscopy (Invited)

L. A. Hughes^{*1}; B. Savitzky¹; H. Deng²; N. Jin²; E. Lomeli²; P. Herring³; W. Chueh²; C. Ophus¹; A. Minor¹

1. Lawrence Berkeley National Laboratory, USA
2. Stanford University, Materials Science and Engineering, USA
3. Toyota Research Institute, USA

Lithium iron phosphate (Li_xPO₄) is a cathode material used in Li-ion batteries that phase separates into Li-rich (LiFePO₄) and Li-poor (FePO₄) regions during delithiation. While these phases are orthorhombic, they have differing chemistry and lattice parameters. The interface that forms between the two phases affects Li-ion transport and over-potential, thereby altering rate performance and life cycle of these batteries. Determining the structure-composition relationship at these interfaces allows for evaluation of underlying mechanisms affecting Li-ion transport. We performed four-dimensional scanning transmission electron microscopy (4D-STEM) to evaluate the lattice parameters as well as scanning transmission X-ray microscopy (STXM) and X-ray ptychography to evaluate the chemistry of pristine LiFePO₄, 50% chemically delithiated LiFePO₄, and FePO₄. Analysis of pixel-by-pixel correlated 4D-STEM and X-ray datasets demonstrates that Vegard's law is obeyed in the mean of the 50% chemically delithiated LiFePO₄ platelets. However, the local region at the interfaces of these 50% chemically delithiated LiFePO₄ platelets show a non-linear evolution of the lattice parameters as a function of %Li. Thus, correlative imaging of Li_xPO₄ platelets reveals invaluable information regarding local chemo-mechanical relationships for elucidation of Li-ion transport mechanisms.

4:00 PM**(EMA-S1-009-2020) Mapping Electric Fields Using Advanced Detectors in Scanning Transmission Electron Microscopy (Invited)**

H. G. Brown^{*1}; Z. Chen³; T. C. Peterson⁴; H. Cheng⁴; N. Shibata²; C. Ophus¹; J. Ciston¹; L. J. Allen³; S. Findlay⁶

1. Lawrence Berkeley National Laboratory, Molecular Foundry, USA
2. The University of Tokyo, Japan
3. Cornell University, School of engineering and applied physics, USA
4. Monash University, Monash Centre for Electron Microscopy, Australia
5. The University of Melbourne, School of Physics, Australia
6. Monash University, School of Physics and Astronomy, Australia

Research into materials for the next generation of computers, batteries and solar cells requires techniques that can characterise both the structural and functional properties of materials, often at atomic resolution. Recently, new developments in segmented detectors and fast readout electron cameras for scanning transmission electron microscopy (STEM) have made it possible to record more detailed information about the interaction of the electron probe with the specimen. This talk will discuss quantitative retrieval of specimen electric fields using precise measurements of electron beam deflection from this data. We explore two different case studies: atomic resolution imaging of atom electric fields in monolayer MoS₂ and thicker samples of the perovskite SrTiO₃, and nanometre scale resolution imaging of the inbuilt electric field of a p-n junction in a GaAs semiconductor sample. Both cases illustrate the experimental challenges of quantitative field measurements in STEM and will be used to discuss the domain of validity of this technique. Finally, this talk will detail challenges for measuring electric fields in strongly correlated functional materials, such as ferroelectrics, as well as strategies to overcome the aforementioned inherent limitations of existing STEM field mapping techniques.

4:30 PM**(EMA-S1-010-2020) Quantifying Octahedral Distortion in Complex Oxide Perovskites with iDPC-STEM**

A. N. Penn^{*1}; A. Kumar²; D. P. Kumah¹; J. M. LeBeau²

1. North Carolina State University, Materials Science and Engineering, USA
2. MIT, DMSE, USA

The versatility of perovskite oxides is enabled by the wide range of suitable A- and B-site cation combinations and the structure's ability to adjust its lattice to accommodate chemical and mechanical stimuli. The distortions and tilting of the oxygen octahedra are not only a structural compensation mechanism of the perovskite, but have also shown to control properties of the material. Therefore accurate atomic structure must be known to determine the origin of material phenomena. X-ray diffraction techniques are prominent for octahedral structure determination, but are limited by spatial resolution and dependable models to refine the structure. Scanning transmission electron microscopy (STEM) enables local atomic structure determination in real space. Here, we will discuss how integrated differential phase contrast (iDPC) STEM allows simultaneous imaging of light and heavy elements without the Z-contrast limitation of annular dark field or aberration-dependent interpretation of other light-element imaging techniques. We will demonstrate how iDPC-STEM imaging can be used to determine octahedral distortions and tilting on the unit cell-to-unit cell basis in bulk and epitaxial thin film perovskite structures. Applications to explaining the atomistic origins of electronic, magnetic, and optical properties of perovskites will also be discussed. This project is funded by NSF DMR-1608656.

4:45 PM**(EMA-S1-011-2020) Investigation of Anti-Phase Boundaries in Ferromagnetic Thin Films using Scanning Transmission Electron Microscopy**

A. Trout¹; I. Pinchuk²; W. Amamou²; R. E. Williams³; R. K. Kawakami²; D. W. McComb^{*1}

1. The Ohio State University, Dept. of Materials Science and Engineering, USA
2. The Ohio State University, Dept. of Physics, USA
3. The Ohio State University, Center for Electron Microscopy and Analysis, USA

A major goal in quantum science is to create a new generation of devices based a spin manipulation. Through spin manipulation, magnetization can be induced in a nonmagnetic material due to close proximity with a ferromagnetic insulator. This is known as the magnetic proximity effect and has been shown to occur in platinum on cobalt ferrite. CoFe₂O₄ is a ferromagnetic insulator with a spinel structure. Spinel oxides have diverse chemical, magnetic, and electric properties, which can be tuned by varying the cation species and coordination environment. The magnetic properties of cobalt ferrite are directly related to the cation distribution and the local microstructure, therefore full characterization of the structure is needed. Here we use high resolution STEM imaging and analytical techniques to investigate the degree of inversion and the presence of anti-phase boundaries (APBs) in CoFe₂O₄ grown via molecular beam epitaxy. It will be shown that APBs have a major influence on the magnetic behavior of the thin film. We will discuss the implications of this and how APBs might be controlled in MBE growth.

5:00 PM**(EMA-S1-012-2020) Visualizations of Complex Charge-Ordered Phases in Colossal Magnetoresistive Manganites (Invited)**

I. El Baggari^{*1}; D. Baek²; B. Savitzky¹; M. Zachman³; R. Hovden⁴; L. Kourkoutis³

1. Cornell University, Department of Physics, USA
2. Cornell University, School of Electrical and Computer Engineering, USA
3. Cornell University, School of Applied and Engineering Physics, USA
4. University of Michigan, Department of Materials Science & Engineering, USA

Manganites, known for the colossal magnetoresistance effect, host charge- and orbital-ordered phases that break the spatial symmetries of the crystal and mediate dramatic property changes including metal-insulator transitions and novel magnetic textures. Many open questions about the microscopic details of charge-ordered states remain. Multiple ground states with different orbital arrangements have been proposed, including site-centered (stripe) and bond-centered order (bi-stripe). These states break different symmetries and are predicted to generate different functionalities. A challenge in probing charge order is its tendency towards short-range correlations, nanoscale coexistence, and incommensurate order. Here we perform cryogenic scanning transmission electron microscopy (cryo-STEM) measurements on manganites. By measuring picoscale lattice distortions at low temperature (93 K), we discover two types of displacement patterns coexisting at the nanoscale. The first is consistent with stripe order and the second represents bi-stripes but with key differences from the idealized model. We visualize intrinsic textures in the ordered state including topological defects and show how they govern long range ordering. These cryo-STEM results highlight the entwined couplings between electronic and lattice degrees of freedom and present a new methodology to probe electron-lattice order.

S2: Advanced Electronic Materials: Processing Structures, Properties, and Applications

Applications of Advanced Electronic Materials

Room: Orange B

Session Chair: Till Frömmling, Technische Universität Darmstadt

10:00 AM

(EMA-S2-001-2020) Large flexoelectric response in ferroelectric ceramics: Mechanisms and potential applications (Invited)

B. Chu*¹

1. University of Science and Technology of China, Department of Materials Science and Engineering, China

It has been found that the flexoelectric response of many ferroelectric ceramics is often several orders of magnitude higher than the theoretically predicted value. The mechanisms for this phenomenon are not fully understood. In this presentation, we demonstrate that there is a spontaneously polarized layer on the surface of ferroelectric ceramics, and this type of surface layer is observed in different ceramic systems, including BaTiO₃, Pb(Zr,Ti)O₃, and Na_{1/2}Bi_{1/2}TiO₃-based ceramics. The piezoelectric response from the polarized surface is one key mechanism for the measured flexoelectric response. We further show that the composition or temperature dependence of the flexoelectric response of the Na_{1/2}Bi_{1/2}TiO₃-BaTiO₃ ceramics can be explained based on the surface mechanism. Finally, the potential applications of the large flexoelectric response of ferroelectric ceramics, including the design of flexoelectric piezoelectric composites, thermal-electrical conversion, and mechanical energy harvesting, will be proposed and discussed.

10:30 AM

(EMA-S2-002-2020) Three-dimensional interconnected ferroelectric ceramic foam-based flexible composites for highly efficient mechanical and thermal energy harvesting (Invited)

G. Zhang*¹; S. Jiang¹; Q. Wang²

1. Huazhong University of Science and Technology, China

2. Pennsylvania State University, USA

Flexible ferroelectric materials are pivotal to various applications including wearable electronic and biomedical devices. Here we report the composites in which the three-dimensional (3-D) interconnected ferroelectric ceramic foams are embedded in the PDMS polymer. Comprehensive mechanical and thermal transfer simulations reveal that the ferroelectric ceramic foams provide a continuous pathway for load and heat transfer to break the load-and-heat-transfer law seen in previous composites that filled with low-dimensional ceramic inclusions. As a result, the developed 3-D composites shows exceptional piezoelectric and pyroelectric responses, thereby enabling concurrent mechanical and thermal energy scavenging. The findings of this work suggest a novel material design for high-performance energy harvesting and self-powered mechanical and thermal sensors.

11:00 AM

(EMA-S2-003-2020) Ultrahigh efficiency relaxor antiferroelectric ceramics for energy storage applications

P. Mohapatra*¹; Z. Fan¹; J. Cui¹; X. Tan¹

1. Iowa State Univ, Mater. Sci. & Eng., USA

Antiferroelectric (AFE) ceramics have high energy and power density owing to the AFE to ferroelectric (FE) phase transformation but suffer from low energy efficiency. The limited efficiency leads to increased energy dissipation and hysteresis loss that can adversely affect device performance in high-frequency capacitor applications. Relaxor materials exhibit near zero electric hysteresis and slim

polarization-field loops. In this work we apply a new strategy of incorporating Bi-based complex perovskites into a base AFE composition of (Pb_{0.97}La_{0.02})(Zr_{1-x-y}Sn_xTi_y)O₃, to introduce relaxor behavior in AFE compounds to enhance their energy efficiency. Among all the compositions, Bi(Zn_{2/3}Nb_{1/3})O₃ is the most effective in inducing dielectric relaxation and minimizing electric hysteresis. It is found that the long-range order of the base AFE material is disrupted by introducing relaxor characteristics showing a diffuse transition between AFE and FE phases and improved energy efficiency. A notable high energy efficiency of 95.6% is achieved at an energy storage density of 2.19 J/cm³ at 115 kV/cm in 0.90(Pb_{0.97}La_{0.02})(Zr_{0.65}Sn_{0.30}Ti_{0.05})O₃-0.10Bi(Zn_{2/3}Nb_{1/3})O₃, which is the highest storage efficiency ever reported in the literature for AFE oxides. This new way of forming “relaxor antiferroelectrics” shows promise to develop new compositions with high energy density and ultra-high efficiency.

11:15 AM

(EMA-S2-004-2020) Recent developments in dielectric cooling based on perovskite ferroelectric ceramics

B. Rozic*¹; A. Bradesko²; U. Plaznik³; B. Malic²; T. Rojac²; Q. Zhang⁴; A. Kitanovski³; Z. Kutnjak⁵

1. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia

2. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia

3. University of Ljubljana, Faculty of Mechanical Engineering, Slovenia

4. Pennsylvania State University, Materials research institute, USA

5. Jozef Stefan Institute, Slovenia

The interest in electrocaloric (EC) effect has been recently revived due to great potential for developing new cooling technologies. Recently, PMN-10PT ceramics have been successfully utilized in a prototype of an electrocaloric cooling device. The recent advances in development of new perovskite relaxor multiferroics with large caloric effects and their use in different solid-state cooling designs will be presented. The effect of electric-energy recovery, the heat regeneration, and the polarization hysteresis losses on the energy efficiency of the system is analyzed. Testing of the cooling device demonstrates the efficient regeneration and establishment of the significant temperature span across the regenerator, exceeding several times the EC temperature change within a single electrocaloric element. The influence of the material's fatigue will also be tested and discussed.

11:30 AM

(EMA-S2-005-2020) Rare Earth Based Multifunctional Perovskite Ceramic Materials for electronic and magnetic applications

D. K. Mahato*¹; D. Singh¹

1. National Institute of Technology Patna (NITP), Physics, India

Electroceramics are advanced ceramic materials that are used in a wide variety of electric, magnetic and optical applications. Electroceramics play essential roles in an ever-increasing extent of the functioning of manufactured products. During the past few years, functional double perovskite ceramic materials have attracted huge attention owing to their multi-disciplinary applications in electronics industry. Different classes of multifunctional double perovskites have gained much scientific interest owing to their rich physics, industrial and technological applications. This functional property can be explored for intelligent sensor, spintronic and functional device applications. In this work, we report the dielectric, electrical and magnetic properties of rare earth based double perovskite ceramics host Zn and Mn. The study of cyclic voltammetry charging discharging plot exhibit its use in supercapacitor and solar cells. The present structural, dielectric and magnetic data make this system for its multiferroic character a promising candidate to various modern functional device applications.

11:45 AM

(EMA-S2-006-2020) Gate-defined Quantum Confinement in few-layer Black Phosphorus TransistorJ. Yang^{*1}; S. Che¹; K. Watanabe²; T. Taniguchi²; S. Moon³; D. Smirnov³; R. Chen¹; C. Lau¹

1. The Ohio State University, Physics, USA
2. National Institute for Materials Science (NIMS), Japan
3. National High Magnetic Field Laboratory, USA

Black phosphorus is a novel two-dimensional(2D) semiconductor which has attracted considerable research interest due to its tunable band gap and high electron mobility. Here we demonstrate quantum confinement defined by split gate in devices based on few-layer black phosphorus. The tunability of split gate can be illustrated by the fact that a device can be tuned off by split gate alone. Quantized conductance is observed when the width of the quantum point contact is varied. In quantum Hall regime, gate-controlled pinching off of quantum Hall states (with filling factor $\nu = -1, -2, -3, -4$) indicates the realization of strong confinement and the potential of manipulation of edge states. The work opens the door for using black phosphorus as platform for electronic and optoelectronic applications.

12:00 PM

(EMA-S2-007-2020) Progress Report for Energy Storage Ferroelectrics: From Bulks to FilmsZ. Sun^{*1}

1. Shaanxi University of Science and Technology, China

Compared with Li ion batteries, fuel cells, and super capacitors, energy storage dielectrics/ferroelectrics have already shown obvious advantages on fast charge-discharge time, providing huge potential on applying in high power devices. Because of their weakness of low energy storage density (ESD), which has been regarded as one of the key factors to determine energy storage materials, commercialization for energy storage dielectrics/ferroelectrics is still far to reach. Motivated by this, developing the ESD of dielectrics/ferroelectrics has been a hot pot in energy storage field and enhancing the dielectric permittivity (ϵ) and electrical breakdown strength (EB) have been considered as two efficient ways. Here, five state dielectric/ferroelectric energy storage materials from bulks to thin films have been introduced with their respective merits and demerits. General methods for improving their ϵ and EB including structure designing, composition optimizing and materials compositing have been revealed, and the superiority for interface engineering has also been pointed out. Finally, energy storage dielectrics/ferroelectrics deserve to have more investigations

Electromechanical Properties and Structure of Bulk and Film Electronic Materials

Room: Orange B

Session Chair: Margo Staruch, US Naval Research Laboratory

2:00 PM

(EMA-S2-008-2020) Critical Role of Residual Stress in Polycrystalline Ferroelectrics (Invited)D. A. Hall^{*1}

1. University of Manchester, School of Materials, United Kingdom

Residual stresses arise in polycrystalline ferroelectrics as a result of inter-granular elastic constraint. Their evolution under thermal, electrical and mechanical loading has a profound impact on functional dielectric, ferroelectric and piezoelectric properties. This presentation will review the origins of residual stresses and their characterisation using x-ray and neutron diffraction methods. Examples will be given to illustrate residual stress development both in traditional lead-based piezoceramics and in recently-developed lead-free materials. Their role in coupling together the ‘intrinsic’

lattice strain and ‘extrinsic’ domain switching contributions to electrostrain will be highlighted. The incorporation of elastic constraint as a central feature in multiscale models of polycrystalline ferroelectrics will also be described. Finally, future prospects for the quantification of residual stresses and improved understanding of their role in the development of ‘thick film’ ferroelectrics will be considered.

2:30 PM

(EMA-S2-009-2020) Ferroelectric and Piezoelectric Properties of Thin Film (1-x)BNKT-(x)SrZrO₃K. M. Grove^{*1}; D. Cann²; B. Gibbons³; S. K. Gupta²; P. Mardilovich⁴

1. Oregon State University, Materials Science, USA
2. Oregon State University, School of Mechanical, Industrial, and Manufacturing Engineering, USA
3. Oregon State University, USA
4. Xaar, United Kingdom

Ceramics based on $(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3-(\text{Bi}_{0.5}\text{K}_{0.5})\text{TiO}_3$ have displayed potential to replace lead-based ceramics in some applications due to their relatively large piezoelectric response. Increases in bulk piezoelectric response have been achieved via the addition of SrZrO_3 as a ternary member in $(1-x)\text{Bi}_{0.5}(\text{Na}_{0.4}\text{K}_{0.6})_{0.5}-(x)\text{SrZrO}_3$. In bulk, this enhancement in piezoelectric response is attributed to a ferroelectric to relaxor transition observed in $(1-x)\text{BNKT}-(x)\text{SrZrO}_3$ between $x=0.02$ and $x=0.03$. To evaluate the impact of SrZrO_3 on thin film piezoelectric properties, chemical solution deposited BNT-BKT-SrZrO₃ films with varying SrZrO₃ content (2.5% to 5%) and BNT-BKT ratios (40BNT-60BKT to 80BNT-20BKT) were synthesized and dielectric, ferroelectric, and piezoelectric response were measured. The enhancement in piezoelectric response between 2% and 3% SrZrO₃ seen in bulk was not observed in thin film embodiments. Initial evidence of the ferroelectric to relaxor transition in thin films was observed in low-field thin film measurements with a reduction in remanent polarization from $0.76\mu\text{C}/\text{cm}^2$ to $0.33\mu\text{C}/\text{cm}^2$ with the addition of 2.5% SrZrO₃. Additionally, the impact of BNT to BKT ratio in BNT-BKT-SrZrO₃ piezoelectric response and microstructure was evaluated. Piezoelectric response increased as BNT-BKT ratios neared 80BNT-20BKT ($d_{33f} = 40\text{ pm}/\text{V}$ in 40BNT-57.5BKT-2.5SrZr and $80\text{ pm}/\text{V}$ in 80BNT-17.5BKT-2.5SrZr).

2:45 PM

(EMA-S2-010-2020) Quantifying Pyroelectric Contributions in PbZr_{1-x}Ti_xO₃ Thin FilmsG. Velarde^{*1}; S. Pandya¹; L. Zhang¹; D. Garcia¹; E. Lupi¹; R. Gao¹; J. Wilbur²; C. Dames²; L. W. Martin¹

1. University of California, Berkeley, Materials Science and Engineering, USA
2. University of California, Berkeley, Mechanical Engineering, USA

Waste-heat energy conversion and wireless power transmission rely on pyroelectrics (a subclass of dielectric piezoelectrics) which exhibit a temperature-dependent polarization. Although dielectric and piezoelectric responses are typically enhanced at chemically-induced phase boundaries, pyroelectric effects have been primarily limited in study to only temperature-induced phase boundaries. Here, we directly identify the magnitude and sign of the intrinsic, extrinsic, dielectric, and secondary contributions to the total pyroelectric response as a function of chemistry across the morphotropic phase boundary (MPB) in thin films of the canonical ferroelectric $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$. Using phase-sensitive frequency and applied dc-bias methods, the various pyroelectric contributions were extracted to elucidate the reduction of the total pyroelectric response at lower Ti concentration. This arises from a combination of decreasing intrinsic response and a sign inversion of the extrinsic contribution upon crossing the MPB. Additionally, the secondary and dielectric contributions span between $-|70-29|$ and $|10-115|\mu\text{C m}^{-2}\text{K}^{-1}$, respectively, following trends in the piezoelectric and dielectric

susceptibility. Finally, the in-plane pyroelectric response is studied for the first time as a function of a-domains within $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ thin films. These findings and methodologies provide insights into the understudied realm of pyroelectrics.

3:00 PM

(EMA-S2-011-2020) Understanding the Structure-Property Relationship in Lead-Free Piezoelectric $[\text{1-x}]\text{Ba}(\text{Zr,Ti})\text{O}_3\text{-}[x](\text{Ba,Ca})\text{TiO}_3$ Through Total Scattering Studies (Invited)

C. M. Culbertson¹; A. Manjon-Sanz¹; D. Hou³; J. L. Jones³; M. Dolgos^{*2}

1. Oregon State University, Chemistry, USA
2. University of Calgary, Chemistry, Canada
3. North Carolina State University, Dept. of Materials Science & Engineering, USA

The piezoelectric material $(1-x)\text{Ba}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3\text{-}x(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ (BZT-xBCT) is currently one of the most promising lead-free piezoelectric materials. However, the local structural response of BZT-xBCT to field is not completely understood. By examining how the local and average structure changes as a function of electric field, the intrinsic contributions and extrinsic contributions to the strain mechanism were deconvoluted. It was found that as the MPB was approached from both the orthorhombic and the tetragonal side of the phase diagram, that the lattice distortion decreased, which allowed increased domain wall motion. At the same time, this increase in the extrinsic contributions suppressed the classical piezoelectric strain, which means that most of the macroscopic piezoelectric response (~70%) at the MPB is derived from domain wall motion. In addition to the in situ E-field study, total scattering studies as a function of temperature using neutron diffraction and EXAFS will be presented. It is important to study these local changes to understand the diffuse phase transition of BZT-xBCT. Preliminary data analysis shows that the local distortions differ from the average structure, where the Zr and Ti local environments are different from each other.

4:00 PM

(EMA-S2-012-2020) Piezo-response force microscopy: From sample preparation to combination with other techniques (Invited)

H. Uršič^{*1}; U. Prah¹; M. Šadl¹; T. Rojac¹; B. Malic¹

1. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia

Piezoelectric ceramics have been extensively studied for sensors, transducers and caloric devices. In these applications, the electric field is applied to the working material in order to induce an electro-mechanical response, which is a complex phenomenon with several origins. Among them is the field-induced movement of domain walls, which is extensively studied using piezo-response force microscopy (PFM). The technique is one of the most frequently applied methods for the characterization of the ferroelectric domains. In this contribution, we will focus on the PFM analysis of ferroelectric bulk ceramics, thick films and nano-sized objects. Flat samples such as thin films do not need special sample preparation, whereas bulk ceramics and thick films need to be properly prepared prior to the PFM investigation. Proper polishing, cleaning and thermal treatment of the ceramic surface are crucial for obtaining high-quality images. On the other hand, nano-sized objects such as plates must be properly fixed to the substrate so they cannot move during scanning. Such pre-analysis treatments will be discussed in the contribution. The second part of the talk will be focused on the combination of PFM with other scanning techniques. The properties of BiFeO_3 -based materials were investigated by combining two or more scanning techniques and the results will be discussed in the contribution.

4:30 PM

(EMA-S2-013-2020) Electronic properties of bismuth iodide (Bi_4I_4) Thin Films

Y. Liu^{*2}; R. Chen²; S. Li¹; X. Liu¹; T. Taniguchi³; K. Watanabe³; B. Lv¹; F. Zhang¹; C. Lau²

1. University of Texas, Dallas, USA
2. The Ohio State University, Department of Physics, USA
3. National Institute for Materials Science (NIMS), Japan

Topological insulator materials have attracted much attention because of their gapless conductive surface states that are protected against perturbations. Bi_4I_4 is a quasi-one-dimensional van der Waals material, and its beta phase has been revealed by angle-resolved photoemission spectroscopy to be a topological insulator, thus offering a new platform for exploring topological phases. To date, all prior works on Bi_4I_4 are based on the bulk material. Here we report transport measurements of thin Bi_4I_4 films that are mechanically exfoliated from bulk crystals. Devices in both alpha and beta phases are characterized. Their gate-tunable resistance demonstrates surface-dominated transport, which is further supported by the observation of weak antilocalization in magnetic fields. Moreover, the increase of the resistance in beta phase below 20K suggests that the inelastic scattering process at low temperature is dominated by the electron-electron interaction.

4:45 PM

(EMA-S2-014-2020) Influencing mechanism of sulfurization temperature on grain growth of $\text{Cu}_2\text{ZnSnS}_4$ thin films prepared by ethanol based solutions

I. Gupta^{*1}; B. C. Mohanty¹

1. Thapar Institute of Engineering and Technology, School of Physics and Material Sciences, India

$\text{Cu}_2\text{ZnSnS}_4$ (CZTS) thin films, synthesized by dip coating solution process, offers a very promising absorber material for thin film solar cells because of its low cost, environmental harmless and earth abundant constituents. While hydrazine based solution processed films have yielded the highest efficiency of ~12.6%, the toxic and carcinogenic nature of hydrazine offsets the advantages. In the context of on-going worldwide research on solution based processing, size of grain has been found to be a crucial factor to fabricate efficient solar cells. In this work, we have prepared phase pure kesterite CZTS thin films of micro-sized large grains by dip coating process from ethanol-based precursor solution followed by sulfurization. The growth of grain size with sulfurization temperature has been studied. The increase in the grain size and uniformity with increase in temperature was observed. The results indicate the promise of the approach for facile growth of good quality films with large grains and hence high photosensitivity.

5:00 PM

(EMA-S2-015-2020) Measuring barrier heights of electrodes with ferroelectric $\text{Hf}_{0.58}\text{Zr}_{0.42}\text{O}_2$ films using internal photoemission (IPE) spectroscopy

M. Jenkins¹; S. Smith²; M. D. Henry²; M. Brumbach²; P. Davids²; J. Ihlefeld³; J. F. Conley^{*1}

1. Oregon State University, School of EECS and Materials Science, USA
2. Sandia National Laboratories, USA
3. University of Virginia, Department of Materials Science and Engineering, USA

Stability, relatively low processing temperature, and compatibility with silicon CMOS materials make HfO_2 based ferroelectric thin films attractive for integration into silicon integrated circuits. The design of devices with integrated ferroelectric HfO_2 layers, such as capacitors, ferroelectric memory, and low power negative capacitance FETs, requires knowledge of metal/ferroelectric electron barrier heights, φ_{Bn} . In the simplest model, $\varphi_{\text{Bn}} = \Phi_{\text{M,vac}} - \chi_{\text{f}}$, where $\Phi_{\text{M,vac}}$ is the vacuum metal work function, χ_{f} is the dielectric electron

affinity. However, this model typically does not hold. In this work, we measure the φ_{bn} between ferroelectric $\text{Hf}_{0.58}\text{Zr}_{0.42}\text{O}_2$ films and various electrode materials using three techniques: x-ray photoelectron spectroscopy (XPS), Kelvin probe, and internal photoemission (IPE) spectroscopy.

5:15 PM

(EMA-S2-016-2020) High-throughput Density Functional Perturbation Theory and Machine Learning Predictions of Infrared, Piezoelectric and Dielectric Responses

K. Choudhary*¹

1. National Institute of Standards and Technology, MML, USA

In this work, combining high-throughput (HT) density functional perturbation theory and supervised machine learning approaches, we explored the territory of compounds with interesting infrared, piezoelectric and dielectric properties. We have computed Γ -point phonons, infrared intensities, Born-effective charges (BEC), piezoelectric (PZ) tensors and dielectric (DL) tensors for 5015 inorganic materials in the JARVIS-DFT database. Analyzing this data, we find 3230 and 1943 materials with at least one far-IR and mid-IR peak, respectively. Similarly, from our computed PZ tensor data, we identify 577 high-PZ materials, using a threshold of 0.5 C/m² as an absolute maximum value. Using a threshold of 20, we find 593 potential high-dielectric materials. Importantly, we analyze the chemistry, symmetry, dimensionality (0D/1D/2D/3D), geometry of materials and several property-correlations to find trends. Finally, we train regression models for the highest IR frequency and maximum BEC, and classification models for maximum PZ and average DL tensors to systematically accelerate materials screening.

S3: Frontiers in Ferroic Oxides: Synthesis, Structure, Properties, and Applications

Ferroelectric and Dielectric Oxides

Room: Magnolia A

Session Chair: Joshua Agar, Lehigh

10:00 AM

(EMA-S3-001-2020) Search and Stabilization of Metastable Ferroelectric Materials: SrHfO₃ (Invited)

L. Garten*¹; S. Dwaraknath²; J. Walker²; J. Mangum³; P. Ndione⁴; Y. Park⁵; D. Beaton⁴; V. Gopalan⁵; B. Gorman³; L. Schelhas⁶; M. F. Toney⁶; S. Trolier-McKinstry⁷; K. Persson⁸; D. Ginley⁴

1. U.S. Naval Research Lab, Material Science, USA
2. Norwegian University of Science and Technology, Materials Science and Engineering, Norway
3. Colorado School of Mines, USA
4. National Renewable Energy Lab, USA
5. Pennsylvania State University, USA
6. SLAC, USA
7. Pennsylvania State University, Materials Science and Engineering, USA
8. University of California Berkeley, USA
9. Lawrence Berkeley National Laboratory, USA

Targeting a particular ferroelectric phase is often complicated by the volatility of the components, the competition between multiple polymorphs, or the metastability of the phase with respect to a centrosymmetric ground state. This work describes how to identify processing routes to stabilize metastable ferroic materials, specifically focusing on the SrHfO₃ system. The P4mm phase of SrHfO₃ was identified from a high-throughput search within the Materials Project as a potential lead-free ferroelectric material. Targeted strain engineering and high frequency deposition were used to preferentially stabilize the P4mm phase over four other lower energy polymorphs of SrHfO₃. A polar distortion with 4mm symmetry is observed in the second harmonic generation polarimetry. The large signal $e_{31,f}$ piezoelectric coefficient is 5.2 pm/V, consistent

*Denotes Presenter

with theory predictions. A clear ferroelectric response is observed in the polarization-electric field loops, positive Rayleigh response and dielectric tunability. This phase of SrHfO₃ is a CMOS compatible, low coercive field, high breakdown strength ferroelectric material.

10:30 AM

(EMA-S3-002-2020) Robust In-Plane Ferroelectricity in Ultrathin Epitaxial Aurivillius Films

E. Gradauskaitė*¹; M. Campanini²; R. Erni²; B. Biswas³; C. Schneider³; M. Fiebig¹; M. D. Rossell²; M. Trassin¹

1. ETH Zurich, Department of Materials, Switzerland
2. Empa, Swiss Federal Laboratories for Materials Science and Technology, Electron Microscopy Center, Switzerland
3. Paul Scherrer Institute, Laboratory for Multiscale Materials Experiments, Switzerland

Layered ferroelectrics, often coined as natural superlattices, exhibit functionalities beyond those of the classical ferroelectric perovskite compounds due to their highly anisotropic structure. Unfortunately, the layered architecture impedes their growth as single-crystalline thin films, and thus their integration into oxide-electronic devices. Here we report epitaxial growth of single crystal, layered Aurivillius Bi₃FeTi₃O₁₅ (BFTO) thin films on a lattice matching NdGaO₃ (NGO) (001)-oriented substrate. We show that growth on a lattice-matched orthorhombic substrate supports the single crystalline form of Aurivillius compounds. A layer-by-layer growth mode is demonstrated, enabling in-situ control of thickness with sub-unit cell accuracy resulting in atomically flat surfaces. The achievement of twin-free films significantly enhances their uniaxial ferroelectric properties. In the ultrathin regime, the films exhibit in-plane polarization with a long-range periodic arrangement of ferroelectric domains with nominally charged domain walls. Ferroelectric hysteresis measurements reveal a remnant polarization of 16.5 $\mu\text{C cm}^{-2}$ and show a remarkable endurance after 10¹⁰ switching cycles. The uniaxial in-plane ferroelectricity of Aurivillius thin films opens up new avenues for alternative device paradigms, less susceptible to limitations arising from the depolarizing field effects in the ultrathin regime.

10:45 AM

(EMA-S3-003-2020) Thickness and strain dependence of piezoelectric coefficient in BaTiO₃ thin films

K. Kelley*¹; R. Vasudevan¹; N. Balke Wisinger¹; S. Kalinin¹; L. Collins¹; D. Yilmaz²; P. Ganesh³

1. Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, USA
2. Pennsylvania State University, USA
3. Oak Ridge National Lab, USA

In recent years, a suite of reports has shown that important ferroic properties of thin films (approximately 30 nm or less) are substantially affected by the strain state, which varies as a function of thickness. A key question that remains is the role of intrinsic as opposed to extrinsic screening on the properties of the thin ferroelectric films, and the precise interplay between strain relaxation and the local electromechanical response. In this work, we use a spectrum of strained to relaxed BaTiO₃ (BTO) thin films grown via pulsed laser deposition (PLD) as a model material system to explore the correlation between interface state and bulk properties. To carefully probe the ferroelectric properties of BTO thin films, we use a combination of band-excitation piezoresponse force microscopy (BE PFM) and interferometric displacement sensing (IDS) resulting in the observation of the d_{33} tensor dependence on thickness. Furthermore, in this work we perform molecular dynamics simulations with a recently developed ab initio derived reactive force-field (ReaxFF) for BTO enabling insight into the causes for the observed relationships with strain and piezoelectric coefficient. These results indicate that the reduced electromechanical coupling likely stems from an interfacial layer of fixed size with unswitchable character ('dead' layer), with correspondingly larger volume fractions for thinner films.

11:00 AM

(EMA-S3-004-2020) Watching ferroelectricity emerging during complex oxide thin film growth in real time (Invited)

M. Trassin*¹

1. ETH Zurich, Department of Materials, 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 therefore accompanying the development of low energy consuming oxide electronics. Epitaxial strain, chemical control on interface atomic termination and charge screening environment tuning are key elements of the ferroelectric domain design. Here we show how nonlinear optics can enable the investigation of the ferroelectric polarization in ultra-thin ferroelectric and multiferroic films during the growth. We find that, the ferroelectric critical thickness and domain state can be addressed in situ during the film deposition. The impact of epitaxial strain, depolarizing field and surface termination on the polar state of ultra-thin films and multilayers are explored in real-time, exempt from substrate contribution. Our work provides direct observation of ferroelectric states during the growth as well as new insights dealing with the physics of ultrathin ferroelectrics and further control of ferroelectric-based heterostructure.

11:30 AM

(EMA-S3-005-2020) Antiferroelectric like structure and photovoltaic effect in BiFeO₃/LaFeO₃ superlattices

M. El Marssi*¹; J. Belhadi¹; S. Yousfi¹; B. Carcan¹; H. Bouyanfif¹

1. Université de Picardie Jules Verne, LPMC, France

Bismuth ferrite (BFO) is the most studied multiferroic due to its robust ferroelectric state coexisting at room temperature with an antiferromagnetic order. Possible cross coupling between both ferroic orders pave the way to so-called MagnetoElectric RAM combining advantages of the ferroelectric and the antiferromagnetic state. A morphotropic phase boundary has been observed in La doped BFO solid solution. Emergence of such MPB is believed to arise from the competition between antiferrodistortive and ferroelectric instabilities. Our approach to investigate the interaction between BFO and LFO is based on superlattices (SLs) that are ideal platforms for exploring antagonistic interactions at the origin of many exotic systems. Cuprates combined with Manganites in SLs were investigated to better understand the competition between magnetic and superconducting orders. Similarly to this strategy we grew series of SLs made of BFO and LFO. Our results indicate an anti-polar structure in the BFO layers that is strongly dependent on the BFO thickness and temperature. Compatibility of the octahedral tilt system seems to be the main driving force for this induced anti-polar state. We have highlighted a switchable PV effect at room temperature. By changing the thickness of the BFO layer we have evidenced a change of PV characteristics from a positive Voc and a negative Jsc to an inverse effect.

11:45 AM

(EMA-S3-006-2020) Exploring Ferroelectric and Photocatalytic Properties of Ba and Mn co-doped Bismuth Ferrite (BiFeO₃) Nanoparticles

A. Dubey*¹; M. E. Castillo¹; S. V. Vladimirov¹; D. C. Lupascu¹

1. University of Duisburg-Essen, Institute for Materials Science, Germany

Multiferroic Bismuth Ferrite (BiFeO₃; BFO) nanoparticles (NPs) are potentially suitable materials for spintronic devices and nano-electronics due to their advantageous magnetoelectric properties at room temperature. We have synthesized Bi_xBa_{1-x}Fe_yMn_{1-y}O₃ (x = 0 – 0.05; y = 0 – 0.05) NPs by a modified wet chemical sol-gel route and characterized them via UV-VIS absorption spectroscopy, photoluminescence (PL) spectroscopy, X-ray diffraction,

high resolution transmission electron microscopy (HRTEM), EDX, impedance dielectric spectroscopy, and piezoresponse force microscopy (PFM). We study the influence of doping on ferroelectric behavior of NPs. We tailored the bandgap of BFO NPs from 2.18 eV to 1.60 eV through doping and explored them as a photocatalyst, in which the methyl orange get degraded faster than in pristine BFO NPs. The dielectric properties and optical characteristics of the Ba and Mn co-doped BFO NPs can be utilized for the development of ferroelectric ultrafast optoelectronic devices.

12:00 PM

(EMA-S3-007-2020) Synthesis of Self-Assembled Room Temperature Multiferroic BiFeO₃-LiFe₅O₈ Nanocomposites (Invited)

Y. Sharma*¹; T. Z. Ward²; A. Chen³

1. Los Alamos National Lab, CINT, USA

2. Oak Ridge National Lab, USA

3. Los Alamos National Lab, USA

In this talk, I will present a new approach to create a robust room temperature multiferroic and will show the first detailed experimental observations of nanoscale phase separation in light element doped functional oxides. I will discuss how the controlled synthesis of lithium (Li) into BiFeO₃ enables the formation of coexisting magnetic and ferroelectric phase composition in bulk ceramic Li_xBi_{1-x}FeO₃, where the resulting multiferroic nanocomposite consists of ferrimagnetic α -LiFe₅O₈ spinel inclusions hosted in a ferroelectric perovskite BiFeO₃ matrix. I will also show how the bulk ceramic pellets can be used as pulsed laser deposition targets to allow synthesis of self-assembled BiFeO₃-LiFe₅O₈ thin film nanostructures, where vertically-aligned LiFe₅O₈ nanopillars are heteroepitaxially embedded in a single crystal BiFeO₃ matrix. First principles calculations support the energetics of phase formation and phase separation that drive the synthesis of these materials. Multimodal imaging methods at various length-scales demonstrate the presence of strong magnetism and ferroelectricity at room temperature in both the bulk ceramics and thin film nanocomposites. I will close by discussing how diverse functional form factors “ceramic and crystalline film” of this novel material could be effective to energy storage, sensing, and memory applications.

Magnetism, Structure, and Defects in Transition Metal Oxides

Room: Magnolia A

Session Chair: John Heron, University of Michigan

2:00 PM

(EMA-S3-008-2020) Order from Disorder in Entropic Oxide Films (Invited)

T. Z. Ward*¹; Y. Sharma¹; A. Mazza¹

1. Oak Ridge National Lab, USA

We will discuss how entropy stabilization is used to create single crystal complex oxide films where one or more cation sublattices are populated by five or more elements. We will give examples of single crystal epitaxial perovskite oxide films containing up to 10 cations. Experimental results from STEM-EELS, XRD, XMCD, neutron diffraction, and SQUID magnetometry will be presented. We find that these materials possess uniform cation distribution throughout the target sublattices, can present a range of charge states on the entropic sublattice, possess magnetic properties which are extremely sensitive to strain anisotropy, and may host long range magnetic order. The ability to populate multiple elements onto a single sublattice in complex crystal structures opens new possibilities for functional design strategies in correlated systems while providing access to fundamental studies seeking to understand how diverse local coupling environments can work to generate macroscopic

responses, such as those driven by electron-phonon channels and complex exchange interaction pathways. This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

2:30 PM

(EMA-S3-009-2020) Antiferromagnetism survives extreme chemical disorder in high-entropy oxides (Invited)

R. Hermann^{*1}

1. Oak Ridge National Laboratory, USA

High entropy oxides are solid solutions stabilized by high configurational entropy. High entropy oxides exhibit several interesting functional properties, such as colossal dielectric constants, superionic conductivity, and low thermal conductivity. Their phase formation and the properties that can emerge from spin order and possible structural instabilities attract much attention. The long range magnetic structure and dynamics in the O rocksalt high entropy oxide ($\text{Mg}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Zn}_{0.2}$) was observed by combining neutron diffraction and inelastic scattering with magnetometry and calorimetry. Neutron scattering reveals that long range magnetic order survives extreme disorder and suggests that short range ordered domains persist even at room temperature. We will discuss the findings related to the long range order and the challenges posed for modelling the dynamics and structure of these disordered system as well as possible avenue for additional characterization. Principal work: Zhang J. J., Yan J. Q., Calder S., Zheng Q., McGuire M. A., Abernathy D. L., Ren Y., Lapidus S. H., Page K., Zheng H., Freeland J. W., Budai J. D., and Hermann R. P., Long-Range Antiferromagnetic Order in a Rocksalt High Entropy Oxide, Chem. Mater. 31, 3705-3711 (2019). Work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

3:00 PM

(EMA-S3-010-2020) Structural and Electronic Phenomena in Jahn-Teller Active Mn Spinel Thin Films (Invited)

R. B. Comes^{*1}

1. Auburn University, Dept. of Physics, USA

Late transition-metal oxides comprised of Ni, Co, and Mn cations are promising materials as catalysts for oxygen reduction and oxygen evolution reactions (ORR/OER). This is particularly true for Co-Mn-O and Ni-Mn-O spinel oxides, which have demonstrated ORR performance comparable to that of more expensive Pt-based materials. Unlike more commonly studied Fe-based spinels, however, the Mn^{3+} ion is Jahn-Teller active in octahedral coordination, which leads to tetragonal distortions in the spinel structure if Mn occupies the octahedral site in the spinel lattice. To study the structural, electronic, and catalytic properties of these spinel oxides, we have synthesized a series of Co-Mn-O and Ni-Mn-O spinel films via oxide molecular beam epitaxy. I will present our work examining the Co-Mn spinel films using x-ray photoelectron spectroscopy, x-ray absorption spectroscopy, and other techniques. These films undergo a strong tetragonal distortion due to the Jahn-Teller effect, opening interesting opportunities for further studies as ferroic materials. Interestingly, we observe very different properties for the Ni-Mn films in comparison to the Co-Mn films due to the strong preference for Ni^{2+} ions to occupy the octahedral site in the lattice. I will also present our electron microscopy and atom-probe tomography studies of spontaneously formed NiMn_2O_4 - Mn_3O_4 nanocomposite films in Ni-deficient Ni-Mn spinels.

4:00 PM

(EMA-S3-011-2020) Electronic and magnetic interplay in entropy stabilized oxide thin films

P. B. Meisenheimer^{*1}; L. Williams¹; S. Sung¹; P. Shafer²; M. Trassin³; R. Hovden¹; E. Kioupakis¹; J. Heron¹

1. University of Michigan, Materials Science and Engineering, USA

2. Lawrence Berkeley National Laboratory, USA

3. ETH Zurich, Switzerland

A unique benefit to entropic stabilization is the increased solubility of elements, which opens a broad compositional space with subsequent local chemical and structural disorder resulting from different atomic sizes and preferred coordinations of the constituents. In the antiferromagnetic entropy-stabilized oxides studied here, we see that by tuning the chemistry, and thus the concentration of local structural distortions, we can either induce or reclaim a large degree of frustration in the magnetic lattice of the material. As the large dielectric response of these materials may be strongly linked to their structure, here we study the interplay of electronic and magnetic functional responses in entropy-stabilized oxides. Our results reveal that the unique characteristics of entropy stabilized materials can be utilized to engineer and enhance magnetic functional phenomena in oxide thin films, as well as offer a powerful platform for the study of defects and functional properties.

4:15 PM

(EMA-S3-012-2020) New Probes for Magnetism Nanoscale Garnets: Insights into Spin-Seebeck-Effect Materials (Invited)

P. G. Evans^{*1}; S. Marks¹; S. Geprägs²; M. Dietlein²; Y. Joly³; M. Dai¹; J. Hu¹; L. Bouchenoire⁴; P. Thompson⁴; T. Schullif⁵; M. Richard⁶; R. Gross²; G. Carbone⁷; D. Mannix⁸

1. University of Wisconsin, Materials Science and Engineering, USA

2. Bayerische Akademie der Wissenschaften, Walther-Meißner-Institut, Germany

3. Institut Néel, France

4. European Synchrotron Radiation Facility, XMaS, France

5. ESRF, France

6. Aix Marseille Université, France

7. MAX IV Laboratory, Sweden

8. European Spallation Source, Sweden

Synchrotron x-ray nanobeam diffraction reveals a diverse magnetic microstructure within emerging materials exhibiting the spin Seebeck effect. Insights into magnetism at the nanoscale in these materials promise to lead to the development of optimized devices through the selection of the local spin polarization. X-ray images of the magnetic domain configuration can be obtained using a new synchrotron nanobeam magnetic diffraction method with structural and elemental specificity, uniquely allowing precise magnetic information to be obtained from nanoscale buried volumes. We report an experimental study of the magnetism within 20-nm-thick gadolinium iron garnet thin film materials within spin-Seebeck-effect devices. The determination of the domain structure closes the loop between microscopic theory and impactful devices and, through combined structural and magnetic sensitivity, extends the potential impact of synchrotron x-ray probes of magnetism into a new regime of scientific applications.

4:45 PM

(EMA-S3-013-2020) Microwave spintronics in magnetic insulators: From fundamental to hybrid systems (Invited)

Y. Li^{*1}

1. Argonne National Laboratory, Materials Science Division, USA

The frontier of high-speed network communications and quantum information calls for novel explorations on solid-state microwave electronics and applications. Magnetic excitations in ferroic materials, or magnons, are good candidates because they are intrinsically

in the gigahertz range, with frequencies tunable via external magnetic field. The abundant physical phenomena in magnetic materials allows their excitations to easily interact with different media, which make them suitable for hybrid and multitasking functionality. We will focus on the thin-film magnetic insulator, yttrium ion garnet. First, we will discuss the fundamentals of its microwave-dynamics detections, including thin films and nanodiscs. Its low damping allows us to drive the magnetic excitations to the deeply nonlinear regime, which reveals new phenomena in dipole-induced nutation modes. Then, we will show the recent progress of magnon-based hybrid system, with examples of magnon-photon coupling on a superconducting resonator and magnon-magnon coupling in a magnetic bilayer thin films. In both cases, the observations of avoided crossing between two disparate excitations suggest their strong coupling, which indicate the potential of coherent communications and information processing. Our results provide new pathways for implementing on-chip magnonic devices with efficient and coherent information processing and transductions.

5:15 PM

(EMA-S3-014-2020) Magnetic Domain Patterns in Isolated and Interacting Islands of Nanofabricated $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$

F. Almonte^{*1}; L. Ortiz¹; D. Sasaki²; J. Song¹; W. Linthicum¹; R. Chopdekar³; Y. Takamura²; B. Huey¹

1. University of Connecticut, Materials Science and Engineering, USA
2. University of California, Davis, Materials Science and Engineering, USA
3. Lawrence Berkeley National Laboratory, ALS, USA

Suitably structured islands of epitaxial LSMO can sustain deterministic magnetic domain patterns due to the interplay between domain wall energies and the crystallographic orientation of structural interfaces. In this work, room temperature Magnetic Force Microscopy is performed to identify such domain patterns for a variety of island shapes and dimensions prepared via masked ion-implantation. Ordered domains predictably spiral around the island center for sub-micron features, while larger structures develop multiple domains with seemingly random directions. Reductive milling furthermore confirms the ability to convert such thin-film magnetic structures into even finer ordered magnetic domain patterns. Finally, magnetic domain patterns are imaged for interacting islands in artificial spin-ice formations.

S4: Complex Oxide Thin Film Materials Discovery: From Synthesis to Strain/Interface Engineered Emergent Properties

Enhanced Functionality through Advanced Synthesis

Room: Orange A

Session Chairs: Elizabeth Paisley, Sandia National Laboratories;
Jon-Paul Maria

10:00 AM

(EMA-S4-001-2020) Hafnium Zirconium Oxide Ferroelectric Performance: Roles of Thickness, Electrode Stress, and Oxygen Vacancies (Pioneer in Synthesis) (Invited)

J. Ihlefeld^{*1}; S. Fields¹; S. Smith²; M. D. Henry³; S. Wolfley²; T. S. Luk²; M. Brumbach²; C. Fancher³; S. T. Jaszewski¹; C. Constantin¹; G. Esteves²; M. Rodriguez²; P. Davids²

1. University of Virginia, Department of Materials Science and Engineering, USA
2. Sandia National Laboratories, USA
3. Oak Ridge National Lab, USA
4. James Madison University, Department of Physics and Astronomy, USA

Hafnium oxide ferroelectrics constitute a potential game changing material for a number of applications, including: Beyond Moore's Law transistors utilizing a negative differential capacitance effect,

highly scaled ferroelectric memory, and infrared sensors and energy harvesters via pyroelectric responses. In this presentation, we will highlight joint activities of the University of Virginia and Sandia National Labs groups to gain understanding of structure-process-property relations of this exciting material. We will discuss how phase assemblage is impacted by material composition and how this affects polarization response, pyroelectric coefficients, and optical second harmonic generation. Next, we will show how thickness scaling results in diminished responses for sub-10 nm thick films, but that artificially high pyroelectric coefficients can be observed for these ultrathin films. The origin of the pyroelectric response is found to be extrinsic in nature and is caused by electrets presumably from charged defects. Finally, we will show efforts to understand how electrode processing affects phase assemblage, film stress, oxygen vacancy concentration, and polarization response.

10:30 AM

(EMA-S4-002-2020) Metal Nitride stress and chemistry effects on polarization and cycling performance of $\text{Hf}_{0.58}\text{Zr}_{0.42}\text{O}_2$ films

S. Fields^{*1}; S. Smith³; M. D. Henry³; S. Wolfley³; M. Rodriguez³; C. Fancher²; G. Esteves³; P. Davids³; J. Ihlefeld¹

1. University of Virginia, Department of Materials Science and Engineering, USA
2. Oak Ridge National Lab, USA
3. Sandia National Laboratories, USA

Atomic layer deposited 20 nm thick $\text{Hf}_{0.58}\text{Zr}_{0.42}\text{O}_2$ (HZO) films between stress modulated 100 nm TaN electrode layers have been evaluated for remanent polarization (P_r), wake-up cycling behavior, and phase assemblage. Through alteration of the background argon pressure during pulsed dc magnetron sputter deposition, the as-deposited stress of the top (bottom) TaN electrode layer has been varied between -1455 and 234 MPa while the bottom (top) TaN electrode stress has been kept near-neutral (-43 MPa). Utilizing $\sin^2(\Psi)$ measurements, the stress state of the ferroelectric HZO following annealing at 600 °C in N_2 for 30 seconds was found to vary between 567 +/- 93 MPa and -387 +/- 73 MPa, respectively. P_r has been observed to positively correlate with increasing HZO tensile stress, varying between 5.6 and 8.5 $\mu\text{C}/\text{cm}^2$. An increasing relative tetragonal/orthorhombic to monoclinic phase ratio has been observed utilizing GIXRD measurements, corroborating electrical characterization trends. The Ta:N ratio of the bottom electrode, determined by x-ray photoelectron spectroscopy, has been determined to correlate with the cycling and wake-up behavior. HZO films between nitrogen starved electrodes required 2.0 MV/cm square wave cycling for the wake-up process occur, while those between nitrogen rich electrodes required 3.0 MV/cm square wave cycles indicating an oxygen-scavenging effect.

10:45 AM

(EMA-S4-003-2020) Ferroelectric Properties of Thin Film $\text{Zn}_{1-x}\text{Mg}_x\text{O}$

J. Hayden^{*1}; J. Maria¹

1. Pennsylvania State University, Materials Science and Engineering, USA

The wurtzite structured $\text{Al}_{1-x}\text{Sc}_x\text{N}$ system exhibits an increasing piezoelectric coefficient with increasing Sc content in the region of substitutional solubility. Recently, $\text{Al}_{1-x}\text{Sc}_x\text{N}$ thin films have been discovered to exhibit ferroelectric hysteresis under exceptionally large coercive fields. The presence of ferroelectricity and enhancement of piezoelectric properties in this system is attributed to a flattening of the potential energy landscape by approaching a metastable layered-hexagonal structure, allowing for easier atomic displacement and switchable polarization. Similarly, ZnO thin films show enhanced dielectric and piezoelectric properties when alloyed with MgO at concentrations that preserve the host wurtzite structure. The present work explores the potential for ferroelectric properties in sputtered $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ (ZMO) thin films near the phase separation region. ZMO thin films with a range of alloying

compositions are deposited by radio frequency magnetron sputtering of composite ceramic targets. X-ray diffraction is used to evaluate the phase purity of ZMO thin films with varying MgO content, and atomic force microscopy is used to study film microstructures and surface morphology. High field electrical polarization measurements are employed to study the room temperature spontaneous polarization in thin film Ir/ZMO/Ir capacitors.

11:00 AM

(EMA-S4-004-2020) Combined Polar Distortion Leading to Ferroelectric Ferromagnet in 1D Tetrahedral Chain Network (Invited)

W. Choi*¹

1. SungKyunKwan University, Physics, Republic of Korea

Transition metal-oxygen (MO_x) polyhedra can be considered as the building blocks of the various material systems of transition metal oxides. The atomic and electronic structures of the transition metal oxides are fundamentally determined by the network of the MO_x polyhedra resulting in emergent functionalities. Particularly, MO_4 tetrahedra with a lower structural symmetry let us further envision a low dimensional network. In this talk, we show the brownmillerite $\text{SrFeO}_{2.5}$ shows a room-temperature ferroelectric ferromagnetic phenomenon via the combined polar distortion of the 1D tetrahedral chain network. The brownmillerite structure possesses 1D ordered oxygen vacancy channels, which can equivalently be viewed as a 1D chain of FeO_4 tetrahedra [1,2,3]. Interestingly, the combined polar distortion of the FeO_4 tetrahedra breaks the structural inversion symmetry leading to the ferroelectricity. Furthermore, the inversion symmetry breaking promotes the Dzyaloshinsky-Moria interaction, realizing a canted ferromagnetism. Hence, the room temperature ferroelectric ferromagnet is presented in the $\text{SrFeO}_{2.5}$ epitaxial thin film [4].

11:30 AM

(EMA-S4-005-2020) Tuning functional properties in manganite heterostructures: Strain or stoichiometry?

A. Chen*¹

1. Los Alamos National Lab, USA

Epitaxial strain has been widely used to tune functional properties in complex oxide heterostructures. Apart from strain effect, a large lattice mismatch also produces other effects including modulations in microstructure and stoichiometry. However, it is challenging to distinguish the impact of these effects from the strain contribution to properties in optimum doped manganite thin films. Here, we use $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3$ (LSMO), a lightly doped manganite close to the vertical phase boundary, as a model system to demonstrate that both strain and cation stoichiometry contribute to functionality tuning. The thinner LSMO films are metallic with a greatly enhanced T_C which is 97 K higher than the bulk value. Such anomalies in T_C and transport cannot be fully explained by the epitaxial strain alone. Detailed microstructure analysis indicates La deficiency in thinner films and twin domain formation in thicker films. Our results have revealed that both epitaxial strain and strain relaxation induced stoichiometry/microstructure modulations contribute to the modified functional properties in lightly doped manganite perovskite thin films.

11:45 AM

(EMA-S4-006-2020) Enhanced magnetism in oxygen deficient $\text{Ga}_{0.5}\text{Fe}_{1.5}\text{O}_{3-\delta}$ epitaxial thin films

H. Kim¹, H. Jeon*¹

1. Pusan National University, Physics, Republic of Korea

Forming oxygen vacancies are often believed to reduce ferroic properties. However, in this presentation we demonstrated changes in magnetism by oxygen contents in $\text{Ga}_{0.5}\text{Fe}_{1.5}\text{O}_{3-\delta}$. (001) $\text{Ga}_{0.5}\text{Fe}_{1.5}\text{O}_{3-\delta}$ (GFO)

epitaxial films were synthesized on (001) YSZ substrates using RF magnetron sputtering. As a comparison, we post-annealed GFO films in 500 Torr of O_2 to fill up oxygens in the lattices. We used x-ray scattering, SQUID magnetometry, and x-ray photoelectron spectroscopy to observe difference in structure, magnetism, and chemistry. We verified oxygen vacancies induce lattice expansion and enhance magnetic moment by the formation of Fe^{2+} and reduction of p-d hybridization. This model study will give a way to control superexchange interaction through control of oxygen vacancy contents.

12:00 PM

(EMA-S4-007-2020) Emergent Novel Functionalities of Ultrathin Freestanding Crystalline Oxide Perovskites (Invited)

X. Pan*¹

1. University of California, Materials Science and Engineering, USA

2D materials such as graphene and transition metal dichalcogenides reveal the electronic phases that emerge when a bulk crystal is reduced to a monolayer. Transition-metal oxide perovskites host a variety of correlated electronic phases, so similar behavior in monolayer materials based on transition metal oxide perovskites would open the door to a rich spectrum of exotic 2D correlated phases that have not yet been explored. Here we report the fabrication of freestanding perovskite films with high crystalline quality almost down to a single unit cell. Using a water-soluble $\text{Sr}_3\text{Al}_2\text{O}_6$ buffer layer, we synthesize freestanding SrTiO_3 and BiFeO_3 ultrathin films by reactive molecular beam epitaxy and transfer them to diverse substrates, in particular crystalline silicon wafers and holey carbon films. We find that freestanding BiFeO_3 films exhibit unexpected and giant tetragonality and polarization when approaching the 2D limit. Our results demonstrate the absence of a critical thickness for stabilizing the crystalline order in the freestanding ultrathin oxide films. The systematic characterization of the cross-sectional samples by atomic resolution transmission electron microscopy reveals that the crystal symmetry and physical properties such as local electrical polarization are strongly dependent on the local strain and boundary conditions of the film.

Advanced Complex Oxide Thin Film Synthesis I

Room: Orange A

Session Chair: Jon Ihlefeld, University of Virginia

2:00 PM

(EMA-S4-008-2020) Defect Chemistry and Reliability in Doped PZT Films

B. Akkopru Akgun¹; W. Zhu¹; C. Randall¹; M. Lanagan²; S. Trolier-McKinstry*¹

1. Pennsylvania State University, Materials Science and Engineering, USA

2. Pennsylvania State University, Dept. of Engineering Science and Mechanics, USA

The processing of lead zirconate titanate is typically conducted under conditions of kinetic control of the lead content; furthermore the absolute lead content is challenging to measure quantitatively. One of the challenges that this imposes is that while the baseline properties depend weakly on the defect chemistry of the interfaces, the lifetime of the devices depends on the compositional profile. As an illustration of this, $\text{Pt/Pb}_{0.99}(\text{Zr}_{0.52}\text{Ti}_{0.48})_{0.98}\text{Nb}_{0.02}\text{O}_3$ (PNZT)/Pt films were investigated. The median time to failure increased from 4.8 ± 0.7 to 7.6 ± 0.4 hours when the top electrode was biased negatively compared to the bottom electrode. This is attributed to (1) a distribution across the film due to PbO non-stoichiometry, and (2) Ti/Zr segregation in PNZT films. The concentration of accumulated near the bottom Pt interface ($6.210^{18} / \text{cm}^3$) after degradation was two times higher than that near the top Pt/PNZT interface ($3.810^{18} / \text{cm}^3$). The accumulation near the bottom Pt/PNZT interface causes severe band bending and a decrease in potential barrier height, which accelerates the electron injection, followed by electron

trapping by Ti^{4+} . Only a small decrease in potential barrier height for electron injection was observed at the top Pt/PNZT interface following degradation.

2:15 PM

(EMA-S4-009-2020) Dynamic Phase Segregation to Avoid High Unstable Ni Valence in Strontium Nickel Oxide Epitaxial Thin Films

L. Wang^{*1}; Z. Yang¹; M. Bowden¹; S. Chambers²; Y. Du¹

1. Pacific Northwest National Laboratory, USA
2. Pacific Northwest National Laboratory, Physical Sciences Division, USA

In our previous study, we prepared a set of $La_{1-x}Sr_xNiO_3$ ($0 \leq x \leq 0.5$) films on (001)-oriented $LaAlO_3$ substrates by oxide MBE and found that Sr doping can significantly enhance the oxygen evolution reaction activity. But the film quality becomes worse when Sr doping level is higher than 50%, presumably because of the high Ni valence state. Although hexagonal perovskite $SrNiO_3$ ($SrNiO_{2.5}$) with Ni^{4+} (Ni^{3+}) can be prepared by synthesis under a high pressure and high temperature condition, the growth of epitaxial $SrNiO_{3-d}$ thin films is still lacking. Here, we have synthesized a set of epitaxial strontium nickel oxide thin films by oxide MBE on $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ (LSAT) (001) substrates. By controlling the Sr/Ni flux ratio as 1:1, in situ RHEED patterns and x-ray diffraction measurements reveal a high degree of structural quality in the $SrNiO_{3-d}$ films. However, in situ XPS measurements show that the Ni is Ni^{2+} . Our further TEM studies clearly show the coexistence of two different phases Sr_2NiO_3 and $SrNi_2O_3$ in the epitaxial $SrNiO_{3-d}$ films, which is consistent with the flux ratio of 1:1 and Ni^{2+} . These dynamic phase segregation during the growth could avoid the high unstable Ni valence and lower the system energy, leading the mixed phases we observed. Moreover, Ni L-edge X-ray absorption spectroscopy (XAS) measurements reveal a large orbital polarization.

2:30 PM

(EMA-S4-010-2020) Defect Structures in $Li_{3x}Nd_{(2/3-x)+(1/3-2x)}TiO_3$ Single Crystal Thin Films

E. Farghadany^{*1}; N. Bagues Salguero²; R. E. Williams²; D. W. McComb²; A. Schirlioglu³

1. Case Western Reserve University, Materials Science and Engineering, USA
2. The Ohio State University, USA
3. Case Western Reserve University, USA

$Li_{3x}Nd_{(2/3-x)+(1/3-2x)}TiO_3$ provides a rich defect structure landscape that is a function of local chemistry and structure including octahedral rotations. In bulk, this leads to self-assembly such as checkerboard structure among many other. In this study, we investigate the structure of the materials under epitaxial growth conditions. Films were grown by pulsed laser deposition (PLD) on $SrTiO_3$ substrates. Deposition conditions namely, substrate temperature, background oxygen partial pressure, and laser energy and pulse frequency were optimized toward epitaxial growth, and was monitored in-situ by reflection high energy electron diffraction (RHEED) method. Various processing parameters include Li content, thickness, and cooling rate. Global structure was characterized by various X-Ray based techniques. Atomic Force Microscopy (AFM) was utilized to study the film surface topography. Transmission Electron Microscopy (TEM) was employed to investigate the local cross-sectional structure of the films. TEM results showed a direct effect of Li content and cooling rate on the formation of different types of defects in the film beyond a critical thickness. In corporation with AFM results, the effects of such defects on the surface morphology was elucidated.

2:45 PM

(EMA-S4-011-2020) Investigating the Intergranular Region of ZnO Varistors via Thin Film Prototypes

K. Ferri^{*1}; R. Floyd¹; S. Lowum¹; E. A. Paisley²; C. DiAntonio²; J. Maria¹

1. Pennsylvania State University, Materials Science and Engineering, USA
2. Sandia National Laboratories, USA

Varistors are technologically important for their large energy handling capabilities and highly nonlinear electrical behavior when voltages above a characteristic switch field are applied. The prototypical $ZnO-Bi_2O_3$ varistor system forms electrostatic Schottky barriers at grain boundaries in response to residual Bi and other dopants left at grain surfaces during Bi_2O_3 segregation. While it is understood that barrier heights can be modulated by varying defect chemistry, there is not yet a complete understanding of the mechanisms by which dopant locations and defect chemistries determine varistor behavior. Bulk studies are challenging due to passive grain boundary formation and difficulties accessing grain boundaries in polycrystalline ceramics. To better understand the $ZnO-Bi_2O_3$ varistor system, we use thin film prototypes to simulate grain boundaries and understand dopant diffusion characteristics, defect chemistries, and grain boundary phase formation. We then correlate this information to mechanisms controlling intergranular barrier heights. For this study, we have investigated as deposited and post-annealed thin film $ZnO//Bi_2O_3//ZnO$ stacks simulating the diffusion, defect chemistries, and electrical properties of bulk ceramic varistors. In addition, we have used conventional ZnO dopants of Co and Mn to modulate phase formation and electrostatic barrier heights within ZnO heterostructures.

3:00 PM

(EMA-S4-012-2020) Tuning Magnetic Anisotropy in Co-BaZrO₃ Vertically Aligned Nanocomposites for Memory Device Integration

B. Zhang^{*1}; J. Huang²; J. Jian¹; B. Rutherford⁴; L. Li³; S. Misra¹; X. Sun¹; H. Wang¹

1. Purdue University, Electrical and Computer Engineering, USA
2. Texas A&M University, Materials Science & Engineering, USA
3. Texas A&M University, USA
4. Purdue University, Materials Engineering, USA

Ferromagnetic nanostructures with strong anisotropic properties are highly desired for their potential integration in spintronic devices. Several anisotropic candidates, such as CoFeB and Fe-Pt, have been previously proposed, but many of them have limitations such as patterning issues or thickness restrictions. In this work, Co-BaZrO₃ (Co-BZO) vertically aligned nanocomposite (VAN) films with tunable magnetic anisotropy and coercive field strength, have been demonstrated to address this need. Such tunable magnetic properties are achieved through tuning the thickness of the Co-BZO VAN structures and the aspect ratio of the Co nanostructures, which can be easily integrated into spintronic devices. As a demonstration, we have integrated the Co-BZO VAN nanostructure into tunnel junction devices and demonstrated resistive switching alluding to Co-BZO's immense potential for future spintronic devices.

Advanced Synthesis II

Room: Orange A

Session Chair: Yingge Du, PNNL

4:00 PM

(EMA-S4-013-2020) Integration of Highly Anisotropic BTO-metal Vertically Aligned Nanocomposite Thin Films on Silicon

M. Kalaswad^{*1}; D. Zhang²; B. Zhang¹; H. Wang²; X. Wang²

1. Purdue University, Electrical and Computer Engineering, USA
2. Purdue University, Materials Engineering, USA

Silicon integration is a crucial step toward low-cost and scalability of vertical nanocomposites, which exhibit fascinating physical properties and various applications. Currently, most vertical

nanostructures are produced by tedious fabrication techniques or on costly substrates. Here, we use pulsed laser deposition (PLD) to successfully demonstrate self-assembled BaTiO₃-Au (BTO-Au) and BaTiO₃-Fe (BTO-Fe) vertically aligned nanocomposites with anisotropic physical properties on buffered Si substrates. The effect of thin (<10 nm) TiN and SrTiO₃ (STO) buffer layers is explored for BTO-Fe films. Detailed microstructural analyses show excellent crystallinity and superior anisotropic magnetic properties for the films grown on a STO / TiN buffer stack. Furthermore, by varying the film growth condition (e.g., ultra-high vacuum and 40 mTorr O₂), the BTO-Au films can be tuned effectively, leading to localized surface plasmon resonance (LSPR) peak and hyperbolic dispersion shift in the visible and near-infrared regime. The integration of these material systems with attractive geometrical and physical property tuning on Si reveals a promising approach to fulfill the potential applications of vertical nanocomposites.

4:15 PM

(EMA-S4-014-2020) Self-assembled ordered three-phase Au-BaTiO₃-ZnO vertically aligned nanocomposites achieved by a templating method

S. Misra^{*1}; L. Li¹; D. Zhang¹; Z. Qi¹; J. Jian¹; M. Fan¹; H. Chen²; X. Zhang¹; H. Wang¹

1. Purdue University, Materials Engineering, USA
2. Los Alamos National Lab, USA

Complex multi-phase nanocomposite designs present enormous opportunities for developing next generation integrated photonic and electronic devices. Here, we demonstrate a unique three-phase nanostructure combining a ferroelectric BaTiO₃, a wide band-gap semiconductor of ZnO and plasmonic metal of Au towards multifunctionalities. By a novel two-step templated growth, a highly ordered Au-BaTiO₃-ZnO nanocomposite in a unique “nanoman”-like form, i.e., self-assembled ZnO nanopillars and Au nanopillars in BaTiO₃ matrix, has been realized, and is very different from the random three-phase ones with randomly arranged Au nanoparticles and ZnO nanopillars in BaTiO₃ matrix. The ordered three-phase “nanoman”-like structure provides unique functionalities such as obvious hyperbolic dispersion in the visible and near infrared regime enabled by the highly anisotropic nanostructures compared to other random structures. Such self-assembled and ordered three-phase nanocomposite is obtained through a combination of Vapor-Liquid-Solid (VLS) and two-phase epitaxy growth mechanisms. The study opens up new possibilities in the design, growth and application of multi-phase structures and provides a new approach to engineer the ordering of complex nanocomposite systems with unprecedented control over electron-light-matter interaction at nanoscale.

4:30 PM

(EMA-S4-015-2020) Tunable Optical Properties in Self-Assembled Oxide-Metal Hybrid Thin Films via Au-Phase Geometry Control: from Nanopillar to Nanodisk

D. Zhang^{*1}; S. Misra¹; L. Li¹; X. Wang¹; J. Jian¹; P. Lu³; X. Gao¹; X. Sun¹; Z. Qi¹; M. Kalaswad²; X. Zhang¹; H. Wang¹

1. Purdue University, Materials Engineering, USA
2. Purdue University, Electrical and Computer Engineering, USA
3. Sandia National Laboratories, USA

Plasmonic oxide-metal hybrid nanostructures exhibit unprecedented optical properties because of the nanoscale interactions between the oxide and metal components. Precise control of the geometry and arrangement of building blocks is key to tailoring system properties towards various nanophotonic applications. In this work, self-assembled epitaxial BaTiO₃-Au nanocomposite thin films with a series of thicknesses are fabricated using a one-step pulsed laser deposition technique. By reducing the film thickness, the geometry of Au phase is effectively tailored from nanopillars to nanodisks, with the aspect ratio (height/width) varied from ~ 4.0 to ~1.0.

The experimental optical spectra and numerical simulation results demonstrate that localized surface plasmon resonance (LSPR) and hyperbolic dispersion wavelength can be effectively tuned in the visible to near infrared regime by varying the film thickness due to the change of Au aspect ratio and free electron density. This study demonstrates a feasible approach in tuning the optical responses in hybrid oxide-metal nanostructures, and opens up enormous possibilities in design and fabrication of novel optical components towards all optical integrated devices.

4:45 PM

(EMA-S4-016-2020) Raman and electronic responses of graphene controlled with ferroelectric domains

B. Dkhil^{*1}

1. Université Paris-Saclay, Laboratoire Structures, France

Graphene (Gr) has attracted tremendous attention in a wide range of fields such as electronics, optoelectronics, spintronics, solar cells, sensors and so on [1]. Usually, graphene sheets are deposited on materials to provide mechanical support. The supporting materials play an important role in improving the properties of Gr layer (e.g. carriers mobility) or even adding new features (n-doped to p-doped transition) due to significant interface effects in such hybrid structures. The polarization reversal characteristic functionality of a ferroelectric (FE) underlayer can be used to tune the carrier concentration and dynamic of graphene layer which can be useful for memory applications [2]. However, one first needs to better understand the mechanisms for the coupling between Gr and FE [3]. Here high-quality Gr film is grown by chemical vapor deposition on a Cu metal substrate and transferred onto BaTiO₃ (BTO) single crystals. Our experiments show there are changes on Gr layer electronic properties correlated to the BTO FE polarization. For instance, we show the so-called 2D graphene second-order Raman mode (related to near zone-edge K and K' optical phonon and thus sensitive to perturbation of the electronic states) displays jumps of its position (up to 20 cm⁻¹) when temperature crosses a ferroelectric phase transitions of BTO which is an indication of a strong modification of the Gr charge density.

5:00 PM

(EMA-S4-017-2020) Designer phonons to sculpt infrared properties

T. E. Beechem^{*1}; E. A. Paisley²; S. Smith²; P. E. Hopkins³; J. Ihlefeld⁴; J. Howe⁴; E. Høglund⁴; J. Matson⁶; T. Folland⁶; J. Caldwell⁶; R. Engel-Herbert⁵

1. Sandia National Laboratories, Optical Sciences, USA
2. Sandia National Laboratories, USA
3. University of Virginia, Mechanical and Aerospace Engineering, USA
4. University of Virginia, Department of Materials Science and Engineering, USA
5. The Pennsylvania State University, Materials Science and Engineering, USA
6. Vanderbilt University, USA

The optical phonons of many oxides manifest through atomic oscillations at infrared frequencies. Often polar, these oscillations create electric fields that themselves have infrared frequencies. When exposed to IR-photons, the electromagnetic and vibration-induced fields can be of similar energy and momentum causing interactions that dominate the material's infrared properties within the Reststrahlen band bounded by the transverse- and longitudinal-optical phonon modes. Thus, by controlling, modifying, and even creating “designer” polar phonons, a route is opened to induce infrared phenomena. Here, the infrared properties of composite oxides composed of lamellar combinations of common dielectrics and ferroelectrics—MgO/CaO and SrTiO₃/CaTiO₃ specifically—are examined to this end. Using a suite of vibrational spectroscopies in combination with materials modelling, the optical response of these “Reststrahlen laminates” extends beyond just a summation of the constituents. The resulting optical properties are examined in light of “synthetic” phonon dispersions that emerge with the

variations in periodicity implicit in lamellar structures. Together, the work suggests a means of creating arbitrary infrared materials via composite phonon responses. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

5:15 PM

(EMA-S4-018-2020) Plasmonic Absorption Tunability in Indium-Doped Cadmium Oxide Thin Films

A. Cleri^{*1}; E. Runnerstrom⁴; J. Nordlander²; J. Tomko³; P. E. Hopkins³; J. Nolen⁵; J. Caldwell⁵; J. Maria²

1. Pennsylvania State University, Materials Science and Engineering, USA
2. Pennsylvania State University, USA
3. University of Virginia, Mechanical and Aerospace Engineering, USA
4. US Army Research Office, USA
5. Vanderbilt University, USA

CdO is one of the most promising candidates for low-loss mid-infrared plasmonics to date, as it demonstrates a tunable range of carrier concentrations, while maintaining high mobilities. These high mobility values enable plasmonic properties with very low loss and very narrow frequency bands. By reactive co-sputtering from metal Cd and In targets using high power impulse magnetron sputtering (HiPIMS) and radio frequency (RF) sputtering respectively, donor-doped CdO thin films with carrier concentrations ranging from 10^{19} to 10^{20} cm⁻³ and mobilities ranging from 300 to 400 cm²/Vs can be readily achieved. Mobility increases with higher In flux, exhibiting a plateau at around 400 cm²/Vs at carrier concentrations between 5×10^{19} cm⁻³ and 1×10^{20} cm⁻³, before dropping slightly at higher carrier concentrations. Optical measurements demonstrate the tunability of near-perfect plasmon absorption across the mid-IR spectral range through varying doping levels. This underscores the utility of doped CdO as a material system for supporting infrared light-matter interactions.

S8: Structure-Property Relationships in Relaxor Ceramics

Local Structure of Relaxors I

Room: Cypress B

Session Chairs: Ian Reaney, University of Sheffield; Yunfei Chang, Harbin Institute of Technology

10:00 AM

(EMA-S8-001-2020) A Hopeless Mess No More: Connecting Structure, Chemistry, and Polarization in PMN-PT Relaxor Ferroelectrics (Invited)

J. M. LeBeau^{*1}; A. Kumar¹; J. Baker²; S. Zhang³; D. L. Irving²; E. C. Dickey²

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. North Carolina State University, Materials Science and Engineering, USA
3. University of Wollongong, ISEM, Australia

Since their discovery nearly 60 years ago, the complexity of nanoscale chemical and structural heterogeneity in relaxor ferroelectrics has made understanding the origins of their unique electromechanical properties a seemingly intractable problem. In this talk, we will discuss how we have employed aberration-corrected STEM to quantify the various contributions of nanoscale heterogeneity in the model relaxor ferroelectric PMN-PT. We identify three main contributions that each depend on Ti content: chemical ordering, oxygen octahedral tilting, and oxygen octahedral distortion. Through application of direct, light element imaging the local polarization we will show that chemical and structural short range order can be connected to polarization fluctuations. Specifically, the heterogeneities are found to act as barriers for long-range polarization alignment, which leads to nanoscale domain formation and

the relaxor response. Furthermore, local monoclinic distortions are found to correlate with the electromechanical performance. Through this approach, the elusive connection between chemical heterogeneity, structural heterogeneity and local polarization is revealed. Results from STEM analysis are used to validate models that can be used to develop the next generation relaxor ferroelectric materials.

10:30 AM

(EMA-S8-002-2020) Branching Bi-displacement directions and nanoscale polar heterogeneities in ferroelectric $K_{0.5}Bi_{0.5}TiO_3$ (Invited)

I. Levin^{*1}

1. NIST, USA

Nanoscale polar heterogeneities are thought to underlie dielectric relaxation in many ferroelectrics and have been recently proposed as a mechanism for enhancing piezoelectric properties. Here we demonstrate the existence of such heterogeneities in the ferroelectric phase of $K_{0.5}Bi_{0.5}TiO_3$ (KBT) which is one of the few known room-temperature tetragonal perovskite ferroelectrics and, as such, a key component in several technologically promising piezoelectric formulations. In the cubic phase of KBT, Bi displacements are found to prefer the $\langle 100 \rangle$ directions and the probability density distribution of Bi features six well-separated sites; a similar preference exists for the much smaller Ti displacements, although the split sites for Ti could not be resolved. The cation displacements are correlated, yielding polar nanoregions, whereas on average, the structure appears as cubic. The cubic \leftrightarrow tetragonal phase transition involves both order/disorder and displacive mechanisms. A qualitative change in the form of the Bi probability density distribution occurs in the tetragonal phase on cooling to room temperature because Bi displacements "branch off" to $\langle 111 \rangle$ directions. This change, which preserves the average symmetry, is accompanied by the development of nanoscale polar heterogeneities that exhibit significant deviations of their polarization vectors from the average polar axis.

11:00 AM

(EMA-S8-003-2020) Local Structure Quantification in the Relaxor Ferroelectric $Ba_5SmSn_3Nb_7O_{30}$

N. Creange^{*1}; M. J. Cabral¹; Z. Yang²; X. Zhu²; X. Chen²; E. C. Dickey¹

1. North Carolina State University, Materials Science and Engineering, USA
2. Zhejiang University, Department of Materials Science and Engineering, China

The complex structures of relaxor ferroelectrics have been studied for decades but recent advancements in aberration-corrected transmission electron microscopy and data analysis are providing new insight into the local structure of these materials. $Ba_5SmSn_3Nb_7O_{30}$ is a relaxor ferroelectric with a tungsten-bronze crystal structure which exhibits an incommensurate modulation, believed to arise primarily from modulations in the octahedral tilting. Insight into local structure distortions and possible correlation with local chemistry is studied via aberration-corrected scanning transmission electron microscopy (STEM). High angle angular dark field images are used to image the cation column positions, while the oxygen atomic column positions are imaged via integrated differential phase contrast (iDPC) imaging. iDPC uses a segmented detector to detect the diffraction pattern center of mass shift as a function of probe position, which is highly sensitive to the electron-wave phase. Quantification of the STEM images is performed by a cross-correlation fit with a 2D gaussian. From this analysis, we quantify atomic-column intensities, distortions, and positions with picometer-scale precision. These local structural features along different zone axes are used to develop a model for the local to long-range structure of this complex relaxor material. This work is partially funded with the NSF Grant No. DGE-1633587.

11:15 AM

(EMA-S8-004-2020) Application of pair distribution function method for characterization of atomic structure in Pb-free dielectric and electrocaloric materialsA. Pramanick*¹

1. City University of Hong Kong, Applied Physics and Materials Science, Hong Kong

Development of new Pb-free relaxor ferroelectrics has received much attention in recent years for application as high-temperature dielectric and electrocaloric materials. Elucidation of composition-structure-property relationships is a prerequisite first step towards rational and efficient design of new materials. Nevertheless, relaxor ferroelectrics are challenging to understand from a scientific viewpoint because of the disordered nature of their atomic structure. For the new Pb-free relaxors, the polar atomic displacements are correlated over only nanometer length scales, although the details of such nanoscale correlations are yet to be fully resolved. In this talk, I will present our recent findings on the nanoscale orderings of polar atomic displacements in the newly designed Pb-free relaxors, which are characterized using pair distribution function analysis of X-ray and neutron total scattering patterns. In addition, I will demonstrate the application of the dynamic pair distribution function (DyPDF) method to elucidate the timescales over which such nanoscale atomic orderings become stable in some Pb-free relaxor systems. The implication of nanoscale atomic ordering and dynamics towards the dielectric, ferroelectric and electrocaloric properties of Pb-free relaxors will be discussed.

11:30 AM

(EMA-S8-005-2020) BaZr_xTi_{1-x}O₃: Lead-free isovalent relaxor ferroelectric or dipolar glassC. Filipic¹; Z. Kutnjak*¹; R. Pirc¹; G. Canu²; J. Petzelt³

1. Jozef Stefan Institute, Slovenia
2. Institute for Energetics and Interphases, National Research Council, Italy
3. Academy of Sciences of the Czech Republic, Institute of Physics, Czechia

Glassy freezing dynamics was investigated in BaZr_xTi_{1-x}O₃ (BZTx) ceramic samples by means of dielectric spectroscopy in the frequency range 0.001 Hz–1 MHz at temperatures 10 < T < 300 K. From measurements of the quasistatic dielectric polarization in bias electric fields up to ~30 kV/cm it has been found that a ferroelectric state cannot be induced in BZT50, in contrast to the case of typical relaxors. This suggests that—at least for the above field amplitudes—BZT50 effectively behaves as a dipolar glass, which can be characterized by a negative value of the static third order nonlinear permittivity. The relaxation spectrum has been analyzed by means of the frequency-temperature plot, which shows that the longest relaxation time obeys the Vogel-Fulcher relation $\tau = \tau_0 \exp[E_0/(T - T_0)]$ with the freezing temperature of 48.1 K, whereas the corresponding value for the shortest relaxation time is ~0 K, implying an Arrhenius type behavior. By applying a standard expression for the static linear permittivity of dipolar glasses and/or relaxors the value of the Edwards-Anderson order parameter $q(T)$ has been evaluated. It is further shown that $q(T)$ can be described by the spherical random bond-random field model of relaxors.

11:45 AM

(EMA-S8-006-2020) Origin of relaxor behaviour in B-site modified barium titanate polycrystalsV. Kaliyaperumal Veerapandiyan*¹; M. Popov¹; P. Groszewicz³; J. Spitaler¹; G. Canu²; V. Buscaglia²; M. Deluca¹

1. Materials Center Leoben Forschung GmbH, Austria
2. National Research Council of Italy, Institute of Condensed Matter Chemistry and Technologies for Energy, Italy
3. Technical University Darmstadt, Faculty of Chemistry, Germany

Relaxors are a sub-class of ferroelectrics with peculiar material properties such as frequency dependent dielectric dispersion and absence of remanent macroscopic polarization. These properties

are relevant for applications in the field of energy storage and telecommunications. In ABO₃ perovskites, relaxor behaviour can be induced by substituting homovalent or heterovalent ions specifically in B crystallographic sites. The charge, ionic size and electronic configuration of the substituent defines the substitution site and induces relaxor behaviour by different mechanisms. In this work, heterovalent (Nb⁵⁺) substituted barium titanate (BNbT) polycrystals were produced and studied to evidence the difference in origin of relaxor behaviour compared to homovalent (Zr⁴⁺) substituted barium titanate solid solutions. Experimental and theoretically modelled Raman spectra (RS) are presented to highlight the peculiarities of BNbT with reference to other systems. Hints on vacancy induced symmetry breaking in Raman spectra of BNbT will be discussed. The extent of lattice disorder is discussed comparing RS results to Nuclear Magnetic Resonance (NMR) spectroscopy. In summary, this multi-scale material characterization approach used here suggests that polar defects in heterovalent-substituted systems trigger a stronger mechanism in disrupting the intrinsic order in the ferroelectric barium titanate lattice.

12:00 PM

(EMA-S8-007-2020) Crystal growth, lattice dynamics and instabilities of BaZrO₃ (Invited)C. Toulouse¹; D. Amoroso²; C. Xin³; P. Veber⁴; M. Ciomaga-Hatnean⁵; G. Balakrishnan⁵; R. Haumont⁶; F. Bourdarot⁷; M. Maglione⁸; P. Ghosez⁹; J. Kreisel¹; M. Guennou*¹

1. University of Luxembourg, Luxembourg
2. CNR-SPIN, Italy
3. Luxembourg Institute of Science and Technology, Luxembourg
4. Institut Lumière Matière, France
5. University of Warwick, United Kingdom
6. Université Paris Saclay, France
7. Institut Laue Langevin, France
8. ICMCB-CNRS, France
9. University of Liège, Belgium

BaZrO₃ is one of the end-members of remarkable perovskite systems: the binary Ba(Zr,Ti)O₃, studied for its relaxor-to-ferroelectric crossover, and the pseudo-ternary (Ba,Ca)(Ti,Zr)O₃, identified as promising for lead-free piezoelectrics. Pure BaZrO₃ has a simple cubic structure down to 2 K, but theoretical DFT studies show that the cubic phase is slightly unstable, with an unstable phonon mode that should give rise to an antiferrodistortive transition driven by octahedral tilts. It has been also suggested that such distortions exist as distorted nano-domains. Besides, BaZrO₃ also exhibits dielectric anomalies in spite of the absence of phase transition. Experimentally, because of its very high melting point, investigations of BaZrO₃ have been mostly limited to polycrystalline samples. Here, we report on the growth and characterization of BaZrO₃ single crystals, and revisit its structure and properties. In particular, we studied the unstable phonon mode by neutron scattering, and performed Raman measurements in a wide range of temperatures and pressures. With the support of detailed calculations of the lattice dynamics, we show that the Raman spectrum does not confirm the hypothesis of distorted nano-domains, but instead can be explained by second-order scattering. The dielectric properties were also measured down to 4.2 K and reveal up to two anomalies, whose origin will be discussed.

Local Structure of Relaxors II

Room: Cypress B

Session Chairs: Kyle Webber, Friedrich-Alexander-Universität Erlangen-Nürnberg; Mojca Otonicar, Jozef Stefan Institute

2:00 PM

(EMA-S8-008-2020) Phase evolution in the ferroelectric relaxor Ba(Ti_{1-x}Zr_x)O₃ from first-principles-based simulations (Invited)

C. Mentzer¹; S. Lisenkov¹; Z. Fthenakis¹; I. Ponomareva^{*1}

1. University of South Florida, USA

We develop and/or use a combination of first-principles density functional theory and first-principles-based effective Hamiltonian approaches to investigate phase evolution in Ba(Ti_{1-x}Zr_x)O₃ ferroelectric relaxor. The simulations reveal two competing effects that arise from the substitution of Ti with Zr and are primarily responsible for the unusual phase evolution and the properties of this family of solid solutions. They are the negative chemical pressure that Zr exerts on the BaTiO₃ matrix and the ferroelectric "inactivity" of Zr itself. The negative pressure has a stabilizing effect on ferroelectricity, the inactivity of Zr disrupts the ferroelectric cooperation. These competing effects are responsible for the pinched phase transition, where the three phases of parent BaTiO₃ merge together, and the loss of ferroelectricity at the onset of relaxor behavior. We trace the origin of the controversial diffuse phase transition to the coexistence of the three ferroelectric phases. In the region of the diffuse phase transition, we detect (polar) nanoregions, which often exhibit unusual nanopillar geometry.

Perovskite/Non-perovskite Relaxors I

Room: Cypress B

Session Chairs: Kyle Webber, Friedrich-Alexander-Universität Erlangen-Nürnberg; Mojca Otonicar, Jozef Stefan Institute

2:30 PM

(EMA-S8-009-2020) What is common between relaxors and dipolar glasses? Are they different? (Invited)

J. Banys^{*1}; S. Svirskas¹; R. Grigalaitis¹; D. Adamchuk¹; J. Macutkevici¹; S. Balciunas¹; D. Jablonskas¹

1. Vilnius University, Faculty of Physics, Lithuania

In this talk I will present the results of the broad band dielectric spectroscopy of relaxors and dipolar glasses. The doping of different ions into BaTiO₃ can lead to very complex behaviour and its receive much attention, both due to fundamental and technological application interests. Rare-earth oxide such Ce, which has intermediate ionic radius between Ba²⁺ and Ti⁴⁺ ions, is an important additive in BaTiO₃-based ceramics for the modification of dielectric properties. The ferroelectric behavior of the Ba(Ti_{1-x}Ce_x)O₃ solid solutions was studied. Dielectric spectroscopy from Hz up to the 40 GHz range and temperature interval 140-500 K was carried out for solid solution ceramics. Ceramics showed a crossover ferroelectric to relaxor behavior. Ba(Ti_{1-x}Ce_x)O₃ solid ceramics doping Ce less than 5% show a weak effect on their dielectric behavior. An increase in the concentration of Ce leads to the fact that three phase transitions of pure BaTiO₃ are compressed into one broad dielectric peak with frequency dispersion. The frequency dependences of relaxation process follows by Havriliak-Negami relaxation, average time relaxation for relaxor ferroelectric follows by the Vogel-Fulcher law. Ceramic of Ba(Ti_{0.8}Ce_{0.2})O₃ is to be considered as a relaxor. Further increase of Ce causes dipolar glass behavior. Obtained results will be compared with dipolar glasses BP/BPI and relaxor PMN.

3:00 PM

(EMA-S8-010-2020) Percolation and Ferroelectric-to-Relaxor-to-Dielectric Crossover in Lead-free Perovskite Solid Solutions (Invited)

Z. Ye^{*1}; J. Zhuang²; A. A. Bokov¹

1. Simon Fraser University, Canada

2. Xi'an Jiaotong University, China

The crossover from normal ferroelectric to relaxor behavior observed due to concentration variation in perovskite solid solutions has been widely studied. The interest is related to the properties of compounds with the compositions close to the crossover point which often show extraordinary dielectric, electrostrictive and piezoelectric performance. Besides, investigations of such materials in which the behavior can be changed from normal to relaxor ferroelectric by comparatively small variation of chemical composition, can provide useful information concerning the mechanisms of relaxor ferroelectricity. Much smaller attention has been paid to another concentration-induced effect, namely the crossover from relaxor ferroelectric to non-ferroelectric behavior. It is expected to be observed in solid solutions of a ferroelectric and a normal dielectric end-members. In the present work we study the relaxor-to-dielectric crossover in the solid solutions of classical ferroelectrics BaTiO₃ and dielectric oxides BaZrO₃, BaHfO₃, BaSnO₃, and DyFeO₃. Experimental techniques of x-ray diffraction, dielectric spectroscopy, piezoresponse force microscopy and measurements of polarization-field hysteresis loops are used. The results are discussed in the framework of percolation theory.

4:00 PM

(EMA-S8-011-2020) Determination of Structure and Property Relationships in the (1-x)NaNbO₃-(x)BaZrO₃ Solid Solution

T. Rowe^{*1}; M. Dolgos¹

1. University of Calgary, Chemistry, Canada

Lead zirconate titanate (PZT) is the industry standard for piezoelectric materials due to its low cost and large piezoelectric response at the morphotropic phase boundary (MPB), which is attributed to polarization rotation. Even with decades of research into finding an alternative, PZT is still largely unmatched, and as such we are attempting to utilize a different mechanism, polarization extension, to synthesize new groups of piezoelectric materials. In this work the (1-x)NaNbO₃-(x)BaZrO₃ solid solution was synthesized. The goal is to obtain a composition dependent polarization extension mechanism while also characterizing the complete structure-property relationships. Thus far, X-ray and neutron measurements show a complete pure phase solid solution with multiple phase transitions until a final cubic transformation near x=0.20. Polarization and strain hysteresis loops show a high strain response corresponding to phase transition near 0.05≤x≤0.10 as well as a transition to a linear dielectric at x=0.20. Dielectric permittivity measurements were also taken over multiple compositions showing a crossover from ferroelectric to relaxor behavior which agrees with the previous property measurements. To summarize, results show an interesting and complex material and further experiments could potentially provide a viable lead-free replacement material.

4:15 PM

(EMA-S8-012-2020) Thermally Induced Phase Switching in Mechanically Biased Single Crystal Relaxors

P. Finkel^{*1}; M. L. Staruch¹; S. Lofland²; S. Young³; E. A. Patterson¹

1. US Naval Research Laboratory, USA

2. Rowan University, Dept. of Physics, USA

3. University of Missouri, Kansas City, USA

In this work we examine the piezoelectric and time-dependent strain response of [011] poled rhombohedral [Pb(In_{1/2}Nb_{1/2})O₃]_{0.24}[Pb(Mg_{1/3}Nb_{2/3})O₃]_{0.44}[PbTiO₃]_{0.32} single crystals under variable

thermal loading. We find that non-uniform thermal flux irradiation incident on a piezocrystal held under mechanical compressive bias stress generates an abrupt jump in strain with a rise time < 1 ms that is much faster than the bulk thermal time scale. This effect is associated with a purely thermally driven weak first-order ferroelectric-ferroelectric rhombohedral-to-orthorhombic phase transition. In situ X-ray diffraction results confirm the phase identification. We demonstrate this transition can be cycled repeatedly with a small thermal hysteresis ($< 3^\circ\text{C}$) under zero applied electric field with a sizable reversible strain jump of $\sim 0.2\%$. Moreover, we show that the thermally driven phase switching behavior can be tuned by varying the bias stress and/or electric field, illustrating the path for establishing effective control parameters and conditions for potential future applications such as actuators, thermally controlled transducers, and sensors. Details of these results on the inter-ferroelectric phase transition and implications to further development of a wide range of devices will be presented.

4:30 PM

(EMA-S8-013-2020) Structure of epitaxial PMN-PT thin films around the MPB (Invited)

U. Gabor^{*1}; I. Rafalovskiy²; N. Daneu³; A. Matavz⁴; V. Bobnar⁴; Z. Samardzija⁵; D. Suvorov³; J. Hlinka²; M. Spreitzer³

1. Peter Grünberg Institute, Forschungszentrum Jülich, Electronic Materials (PGI-7), Germany
2. Institute of Physics of the Czech Academy of Sciences, Department of Dielectrics, Czechia
3. Jozef Stefan Institute, Advanced Materials, Slovenia
4. Jozef Stefan Institute, Condensed Matter Physics, Slovenia
5. Jozef Stefan Institute, Nanostructured Materials, Slovenia

$\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$ is a relaxor-based ferroelectric material that exhibits interesting dielectric and piezoelectric properties. Especially complex domain architectures are formed in compositions around the morphotropic phase boundary. The polar structure of thin films is additionally affected by the epitaxial strain. In order to understand the structure of these films, multi-scale analysis is called for. Limitations of individual analysis techniques will be discussed. At the same time, it will be presented how a combination of high-resolution X-ray diffraction, selected area electron diffraction, atomic-resolution scanning transmission electron microscopy, polarized Raman scattering and wavelength-dispersive X-ray spectroscopy can be used to elucidate the structure of this material. Furthermore, it will be shown how macroscopic piezoelectric and dielectric measurements in different configurations can aid in understanding the structure of the films. Growth-related aspects will also be discussed, with emphasis on the challenges and peculiarities occurring in the growth of films with volatile components. Routes for the preparation of single-phase films with near-nominal stoichiometry will be presented, along with the specific defects that appear with off-stoichiometry. The role of the substrate on the phase purity and film quality will also be discussed. It will be shown why in some cases a rough interface is preferred.

S10: Point Defects and Transport in Ceramics

Predictive Point Defect Energetics and Equilibria from Density Functional Theory and other Computational Methods

Room: Citrus A

Session Chair: Elizabeth Dickey, North Carolina State University

10:00 AM

(EMA-S10-001-2020) Data Driven Pathways to Computationally Fast and Scientifically Accurate Models For Surfaces and Interfaces in Ionic Solids (Invited)

D. S. Mebane^{*1}

1. West Virginia University, Mechanical and Aerospace Engineering, USA

Surfaces and interfaces dominate the electrical and electrochemical properties of ion-conducting ceramics. However, the most common continuum-scale theoretical treatments rely on dilute-case assumptions: the quantitative predictions of these theories have been shown to be at odds with microscopic experimental observations. Concentrated systems are dominated by interactions among constituent ionic defects and any quantitative continuum theory must take interactions into account. While the physics of every interface will be unique and must be considered individually, we have proposed a general theoretical framework that will account for defect interactions at surfaces and interfaces. The phenomenological yet physical framework includes data-driven methods for discovering the functional form of excess free energies using Bayesian inference-based machine learning tools. The framework will be presented along with applications to surfaces and grain boundaries in acceptor-doped ceria.

10:30 AM

(EMA-S10-002-2020) Beyond the Brouwer approximation: Point defects in oxides from first principles (Invited)

D. L. Irving^{*1}; J. Baker¹; P. C. Bowes¹; Y. Wu¹

1. North Carolina State University, Materials Science and Engineering, USA

First principles approaches, informatics, and artificial intelligence are emerging as next generation tools for materials discovery and design. While there has been significant focus on using these tools in the identification of new materials, there has been less of a focus in using these tools for the realization of optoelectronic properties through defect engineering. Defects are not only central to these properties but they also present one of the most significant obstacles in going from discovery to applications in the optoelectronic space. In this talk, results obtained from a new suite of point defect informatics tools that have been developed to address this issue will be presented. Predictions from this toolset will be applied to an array of wide bandgap materials. Predominantly, the study and design of ceramic grade dielectric materials (SrTiO_3 and BaTiO_3) will be discussed, but the application of this toolset to a wide band gap semiconductor system (AlN) will also be shown. These results will be highlighted and compared to companion experimental measurements or data from the literature. Extension of the toolset to address multiscale/multiphysics engineering spaces (e.g. polycrystalline and electronic devices) will also be briefly discussed.

11:00 AM

(EMA-S10-003-2020) First Principle Studies of Point Charge Defect in Phosphorene

B. Rijal^{*1}; A. Z. Tan¹; R. G. Hennig¹; C. Freysoldt²

1. University of Florida, Materials Science and Engineering, USA
2. Max-Planck-Institut für Eisenforschung GmbH, Germany

Vacancies, adatoms, dopants, and interstitials change the electronic and optical properties of materials and also have been proposed as qubits for quantum computing. These defects can be charge neutral; however, some defects can have a net charge. The computational modeling of formation, migration, and reactions of charged defects will allow us to study doping of materials in the newly discovered family of two-dimensional materials for use in electronic devices. The theoretical study of charged defects presents challenges and introduces electrostatics artifacts. In this study, we calculate formation energies of charged defects in two-dimensional black phosphorus using correction method that is based on a surrogate model for the electrostatics. We found that the neutral phosphorus vacancy is the most stable state in the band gap region.

11:15 AM

(EMA-S10-004-2020) Simulation studies of oxygen diffusion in Sr-doped LaMnO₃

J. M. Börgers^{*1}; R. A. De Souza¹

1. RWTH Aachen University, Institute of Physical Chemistry, Germany

Mixed-valence manganites are very promising candidate materials for resistive switching due to the possibility to generate multilevel resistance states as well as area-dependent switching. This enables their use in future non-volatile memories or novel neuromorphic circuits. The aim of our work is to gain a deeper understanding of the microscopic mechanisms of resistive switching in mixed valence manganites with the focus on Sr-doped LaMnO₃ ((La_{1-x}Sr_x)MnO_{3±δ}, LSMO). It is widely accepted that ionic transport plays an important role in the field of resistive switching. Due to the presence of grain boundaries (GBs) in technologically-relevant CMOS-compatible polycrystalline manganite devices and the knowledge that GBs significantly influence the ionic transport, the investigation of the impact of GBs on resistive switching is of special interest. In this study, we focus on investigating ionic transport in LSMO as well as along grain-boundaries in bicrystals of LSMO by Molecular Dynamics simulations, employing empirical pair potentials. In particular, the effect of Sr acceptor dopants, cation antisite defects and cation vacancies on oxide-ion transport is examined.

11:30 AM

(EMA-S10-005-2020) Grain size-dependent conductivity of Al-doped SrTiO₃ from multiscale simulation

Y. Wu^{*1}; P. C. Bowes¹; J. Baker¹; D. L. Irving¹

1. North Carolina State University, Materials Science and Engineering, USA

Strontium titanate, or STO, as a ceramic grade dielectric material is used in a wide range of electronic components, e.g. varistors, capacitors, and memristors, whose electrical response is governed by the ensemble of lattice point defect introduced during doping. Often in these applications, STO polycrystals are used instead of single crystals due to the reduction in cost and partial mitigation of STO's degradation lifetime. Therefore, an understanding and exploitation of structure-property-processing relationships are required to facilitate the tailoring of the electrical response of these materials. To this end, a grand canonical multiscale space-charge model has been developed here to explore the critical role of grain boundaries in predicting the emergent electrical properties. This model combines a database of point defect properties from state-of-the-art hybrid exchange-correlation density functional theory calculations

with finite-element simulations of the internal electric field and its coupling to defect redistribution and reionization processes throughout the grain. It is applied to simulate the electrical conductivity of polycrystalline aluminum-doped STO at different grain sizes and oxygen partial pressures. The simulated results are compared with experimental measurements from the literature. The underlying defect mechanisms and local conductivities will be discussed.

11:45 AM

(EMA-S10-006-2020) Modeling Space Charge Control of the Spin States of the Oxygen-Vacancy Complex in AlN

P. C. Bowes^{*1}; Y. Wu¹; J. Baker¹; D. L. Irving¹

1. North Carolina State University, Materials Science and Engineering, USA

The development of impurity point defect based quantum information systems has been hampered by the fact that the desirable spin states of the defects are often unstable for Fermi levels obtained at increased impurity concentrations. One example of this problem is the complex between an aluminum vacancy and oxygen impurity on a neighboring nitrogen site in AlN, $v_{Al}-1O_N$. The neutral complex ($v_{Al}-1O_N$)⁰ is predicted to be stable for Fermi levels (μ_e) below midgap and have a spin triplet configuration. However, defect equilibrium simulations presented in this work show $v_{Al}-1O_N$ is unstable relative to isolated oxygen impurity defects for μ_e below midgap, and forms as ($v_{Al}-1O_N$)⁻² for μ_e above midgap. As a potential solution to this problem, the space charge perturbed defect chemistry near the interface of a Si/Mg:AlN homojunction was simulated. The results showed ($v_{Al}-1O_N$)⁰ can be stabilized within 6 nm of the interface in the Si-doped portion depending on the processing conditions. Such control is critical to realizing point defect based quantum information systems.

12:00 PM

(EMA-S10-007-2020) Electrochemical proton intercalation for energy efficient neuromorphic computing (Invited)

B. Yildiz^{*1}

1. Massachusetts Institute of Technology, USA

The goal of this research is to design an all solid inorganic device that serves as an analog synapse via resistive switching based on proton intercalation, for accelerating machine learning. Simultaneously, we advance the scientific understanding of mechanisms and kinetics governing the resistive switching in this mode. Cation intercalation is an attractive resistive switching mode that has the potential to have energy consumption per synaptic event that is comparable to or even lower than that in the brain. We are developing a 3-terminal device based on H⁺ cation (proton) intercalation, in scalable and CMOS-compatible oxides, should be the most promising compared to other cations. Hydrogen has the smallest ionic radius and the highest cation mobility that should improve the device energy efficiency (lower voltages needed to shuffle protons between electrodes, and faster switching speeds). We have demonstrated one such device, using a solid state hydrogen source, a solid electrolyte and a proton-induced resistive switching oxide. The switching properties demonstrated low energy, symmetric potentiation, very high off/on resistance ratio, hundreds of states, and small change in open circuit potential. We have assessed the resistive switching mechanism of the active oxide by using x-ray photoelectron and absorption spectroscopy and first principles calculations.

Structure and Mobility of Defects and Defect Complexes

Room: Citrus A

Session Chair: Elizabeth Dickey, North Carolina State University

2:00 PM

(EMA-S10-008-2020) There is no Fe⁴⁺: What X-Ray spectroscopy can tell you about point defects (and what not) (Invited)

D. N. Mueller*¹

1. Forschungszentrum Juelich, Peter Gruenberg Institute, Germany

Charged point defects are an integral part of defect equilibria in solid state ionics, especially when reactions with a gas or liquid are involved. With the advent of X-ray spectroscopic methods made possible in atmospheres approaching ambient pressure and at elevated temperatures it has become tempting to observe these ions and their charge states directly as surface and bulk redox processes take place. Though with the right checks and balances this approach can give, and has given, invaluable insights into mechanisms governing electrochemical properties of solids and their interaction with gases and liquids, it has also led to many misconceptions. In this presentation, I will use prototypical materials such as (La,Sr)(Fe,Co)O_{3-δ} and Sr(Ti,Co)O_{3-δ} utilized in solid state electrochemistry to showcase the strengths and limitations of in situ X-Ray absorption (XAS) and photoemission spectroscopy (XPS). The secession from using XAS and XPS to (attempt to) simply determine formal oxidation states as a function of temperature, chemistry and atmosphere has, for example, led to recognition of the role of the transition metal in the perovskite structure in the former and peculiarities in the conduction mechanism of the latter compound.

2:30 PM

(EMA-S10-009-2020) In situ optical absorption as a probe of defect equilibria and kinetics in oxide thin films (Invited)

E. Skiba¹; H. Buckner¹; T. Chen³; N. Kim²; E. Ertekin²; N. H. Perry*¹

1. University of Illinois at Urbana-Champaign, Materials Science & Engineering, USA
2. University of Illinois at Urbana-Champaign, Mechanical Science & Engineering, USA
3. Kyushu University, I2CNER, Japan

The oxygen non-stoichiometry of oxide thin films, particularly under operating conditions of interest, can be difficult to measure. Similarly, there exist few techniques that can interrogate oxygen surface exchange kinetics in a contact-free, continuous, and in situ manner – necessary for insight into the native surface behavior and degradation. In situ optical transmission measurements enable determination of both of these quantities, which are central to efficiency and lifetime of operating devices. In this talk, I will focus on their application to mixed ionic and electronic conductors (MIECs). High temperature electrochemical pumping studies combined with density functional theory simulations have demonstrated how the subgap absorption is proportional to oxygen content in the MIEC Sr(Ti,Fe)O_{3-x} under oxidizing conditions. On this basis, we have applied optical transmission relaxation (OTR) to study the surface exchange kinetics of this and related MIEC thin films before, during, and after crystallization. Simultaneous OTR and electrical conductivity relaxation measurements yield the same results. We find dramatic enhancements in oxygen surface exchange kinetics upon in situ crystallization and are now seeking to understand the underlying, possibly causative, changes in point defect chemistry through optical, X-ray absorption, and electrical conductivity measurements.

3:00 PM

(EMA-S10-010-2020) Atomic Scale Microscopy of Point Defects and Their Complexes in Beta-Ga₂O₃

J. Johnson¹; H. Huang¹; J. Hwang*¹

1. The Ohio State University, Materials Science and Engineering, USA

Point defects are at the heart of the important properties of wide band-gap and oxide semiconductors, and therefore understanding the details of point defects and their role in determining the properties becomes imperative. b-Ga₂O₃ has received significant attention recently due to its unique advantages, including high breakdown voltage and availability as bulk substrates, which make it a viable candidate for next-generation power device applications. We present the first direct microscopic observation of the formation of interstitial-divacancy complexes within b-Ga₂O₃ lattice using atomic resolution scanning transmission electron microscopy. We observed that cation atoms are present in multiple interstitial sites, and each interstitial atom is paired with two adjacent vacancies. The observed structure of the complexes is consistent with the calculation using density functional theory, which predicts them to be compensating acceptors. The number of the observed complexes increase as a function of Sn doping concentration, which matches with the increase in the concentration of the trap state at E_c - 2.1 eV measured using deep level optical spectroscopy, which strongly suggests that the defects corresponds to that trap level. Our finding provides new crucial information on the exact structural origin of the properties of b-Ga₂O₃ that has been unobtainable using other methods.

3:15 PM

(EMA-S10-011-2020) Oxygen partial pressure dependence of electrical conductivity in Fe-doped Ga₂O₃ single crystal

G. Ryu*¹; P. Reddy¹; R. Collazo¹; E. C. Dickey¹

1. North Carolina State University, Materials Science and Engineering, USA

Gallium oxide (Ga₂O₃) has attracted attention due to its wide band gap, high breakdown voltage and tunable electrical properties, and n-type or semi-insulating electrical behavior can be respectively achieved by Sn (Si) or Fe dopants. While many studies have contributed to a fundamental of electrical conduction in n-type Ga₂O₃, the origin of semi-insulating properties of Fe-doped Ga₂O₃ is less well studied especially with respect to the interplay between the dopant and the intrinsic lattice defect chemistry. In this work, we investigate the oxygen partial pressure (pO₂) dependence of the electrical conductivity of Fe-doped Ga₂O₃ single crystals to provide insight into the intrinsic lattice defect chemistry of Ga₂O₃. 4-point DC electrical conductivity was measured in relatively high pO₂ range from 10⁻⁴ to 10⁰ atm. The crystal was electrically and thermally equilibrated as a function of time at each temperature and pO₂ condition. AC impedance spectra were measured and fitted to an equivalent circuit model and the bulk conductivity contribution compared to the DC measurements and prior literature. Hall measurements were also conducted to attain the hall carrier density and mobility. Finally, the experimental results were interpreted from a view point of point defect chemistry and its relation to electrical conduction.

4:00 PM

(EMA-S10-012-2020) Concentration and mobility of defects in rare-earth substituted ceria: Effects of strain, interfaces, and defect association (Invited)

G. Harrington*¹

1. Kyushu University, Center for Co-Evolutional Social Systems, Japan

Mechanically confined systems such as thin films are an ideal platform for investigating the electro-chemo-mechanics of electroceramics, and rare-earth substituted ceria is an excellent model material to study these effects. In this presentation, we discuss two key experimental findings. First, we demonstrate that the migration

barrier in rare-earth substituted CeO_2 can be modified by lattice strain. Using an unconventional approach to straining films, we developed a quantitative consensus on the variation in the transport properties of ceria as a function of lattice strain. We also experimentally demonstrate the effects of migration direction with respect to the biaxially strained plane. We find that the modification is dependent on the size of the dopant cation, showing that defect association plays a substantial role. Second, we explore the extent that charge carrier concentrations a mixed ionic-electronic conductor (MIEC), Pr substituted CeO_2 (PCO), can be modified at interfaces. By engineering the density and proximity of interfaces in PCO/ SrTiO_3 multilayers, we demonstrate a lowering in the effective enthalpy for Pr reduction, allowing the non-stoichiometry and density of charge carriers to be tailored.

4:30 PM

(EMA-S10-013-2020) Transport and surface exchange properties of n-type mixed conductors (Invited)

H. Takamura*¹

1. Tohoku University, Department of Materials Science, Japan

Surface oxygen reduction reaction (ORR) rates at n-type oxide-based mixed ionic–electronic conducting (MIEC) solid oxide fuel cell (SOFC) cathodes can be expected to be enhanced relative to that at p-type MIEC cathodes due to the greater availability of electrons at higher energies in the band structure needed for the charge transfer reaction. However, given the difficulty of achieving coexisting oxygen vacancies and electrons in the conduction band under oxidizing cathode conditions, no stable n-type MIEC cathodes have been reported to date. In this study, a predominantly n-type MIEC conductivity is confirmed in a Ba–In-based oxide (BNIM) co-doped with Nd and Mn at high temperature and high $P(\text{O}_2)$ confirmed by the $P(\text{O}_2)$ dependence of the electrical conductivity and negative Seebeck coefficients, combined with readily measurable oxide ion transference numbers. This coexistence of n-type electronic and oxide ion conductivities is discussed based on the electrical behavior of BNIM with different Mn levels and is attributed to the significant change in the degree of anion Frenkel ordering and the band structure associated with heavy donor doping of $\text{Ba}_2\text{In}_2\text{O}_5$. This novel n-type MIEC has the potential for enhancing the ORR at SOFC cathodes at reduced temperatures and thereby identifying new potential candidate cathode materials for next-generation SOFCs. Their surface exchange kinetics will be also discussed.

5:00 PM

(EMA-S10-014-2020) Effects of Electrode Composition and Potential on Moisture Incorporation and Degradation of Dielectrics and Piezoelectrics

J. McGarrahan*¹; E. C. Dickey¹

1. North Carolina State University, Materials Science and Engineering, USA

The time-dependent properties of dielectric and piezoelectric materials in humid environments is an important performance metric, as humidity-related degradation can dominate device lifetime in some applications. The effect of proton incorporation is a major motivation for conducting this research. This project aims to measure surface exchange and diffusion kinetics of OH^- and H^+ in commercially relevant ceramics: BaTiO_3 and SrTiO_3 in relation to multilayer ceramic capacitors. The work focuses on tracer diffusion studies using deuterated water, and in some cases ^{18}O -enriched water, to study incorporation pathways, mechanisms and kinetics of H^+ and OH^- in dielectric devices. Specifically, the relationship between acceptor doping and proton incorporation will be presented, as well as comparing ion incorporation in nominally undoped BaTiO_3 and SrTiO_3 .

5:15 PM

(EMA-S10-015-2020) Ion Transport in SrTiO_3 antiphase boundaries

J. Kler*¹; R. A. De Souza¹

1. RWTH Aachen University, Institute of Physical Chemistry, Germany

The cubic perovskite strontium titanate (SrTiO_3) can accommodate small deviations from nominal cation stoichiometry $0.995 \leq \text{SrO}/\text{TiO}_2 \leq 1.002$. For $\text{SrO}/\text{TiO}_2 < 0.995$, TiO_2 is exsolved as a second phase. Ruddlesden and Popper found that for $\text{SrO}/\text{TiO}_2 > 1.002$ the excess is accommodated by the formation of $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$ phases. These Ruddlesden-Popper phases consist of alternating TiO_2 and SrO layers with an additional rock-salt layer every n th SrO layer. During the pulsed laser deposition of Sr-rich SrTiO_3 thin films, the formation of Ruddlesden-Popper-type antiphase boundaries (APB) are observed. After a current is applied to these thin films, the formation of SrO islands at the surface along the APB are observed. In order to understand this behavior, high order ($n = 10$) R-P phases are used as a model system in which to examine ion transport in antiphase boundaries (APB) in SrTiO_3 . Static atomistic simulations, employing various sets of empirical pair potentials, are used to examine the formation energies of oxygen and strontium vacancies in R-P phases. In addition, the activation energies of oxygen-vacancy and strontium-vacancy migration are studied. Lastly, molecular dynamic (MD) simulations were carried out to determine the strontium diffusivity in bulk SrTiO_3 and in the APB.

S12: Electronic Materials Applications in 5G Telecommunications

Industry and 5G

Room: Cypress C

Session Chairs: Geoff Brennecke, Colorado School of Mines; Nate Orloff, NIST

10:00 AM

(EMA-S12-001-2020) What is 5G and how can materials help?

N. Orloff*¹

1. NIST, Communications Technology Laboratory, USA

The fifth generation (5G) of cellular telecommunications technology differs from earlier generations in several meaningful ways, but the biggest differences are in targeted data rates (> 10 gigabits/second) and lower latency (< 1 millisecond) communications. Perhaps the most exciting areas of 5G are the new mm wave bands, which require innovations in both hardware and software. These new hardware innovations push the limits of what is possible at foundries with conventional materials. As a result, 5G handsets have thus far exhibited overheating and poor performance. To solve the problems in 5G, electrical engineers are more frequently looking to the materials community to engineer new materials to target specific applications. In this presentation, we will discuss 5G and how materials can help.

10:15 AM

(EMA-S12-002-2020) Evolution of RF content and the challenges of developing complex RF modules and first filter prototypes for 5G (Invited)

R. Rothmund*¹

1. Qorvo, USA

With 5G NR standards on the horizon, ultra-wide high frequency bands will need to be addressed. BAW is well suited for the new radio bands below 6 GHz requiring rejection and steep transitions. Many of the new bands feature an exceptionally wide passband which calls for larger coupling coefficients than traditional thin-film piezoelectric layers provide. The presentation gives an updated overview and describes recent trends for high frequency bands, wide bandwidth

filters, miniaturization and thermal management. The evolution of RF content and the challenges of developing complex RF modules and first filter prototypes for 5G are discussed.

10:45 AM

(EMA-S12-003-2020) Novel Low Dielectric Constant, High Q, Temperature Compensated Microwave Dielectric System for 5G mm-wave based Applications (Invited)

M. D. Hill¹; S. Polisetty¹; D. Firor²; H. Hancock³; D. Cruickshank¹

1. Skyworks RF Ceramics (Trans-Tech Inc.), Research and Development, USA
2. Skyworks RF Ceramics, (Trans-Tech Inc.), New Product Development, USA
3. Skyworks Ireland, Research and Development, Ireland

It is well known that 5G Communications will use two distinct frequency bands: 3-6 GHz (sub-6) and mm-waves (20-100 GHz). The types of devices, and hence the materials required, will be different for these two frequency ranges. Temperature stable dielectric materials with low dielectric constants (< 15) and ultra-low loss tangents will be enabling materials for mm-wave filtering applications as well as for substrates for co-firing with other functional materials to create integrated devices. Recently, a family of materials has been discovered which meets these criterion while firing at temperatures below 1400 C. The crystal chemistry and phase equilibria for this material system are presented along with the significant microwave dielectric properties. Preliminary data relevant to co-firing this material with other magnetic materials are also presented.

11:15 AM

(EMA-S12-004-2020) High performance ultra-thin alumina ribbon ceramics and multilayer RF devices (Invited)

C. Zhuang¹; N. Z. Zhelev¹; C. Kim¹; S. Seok¹; H. Kim¹; W. Bouton¹; M. Badding¹

1. Corning Incorporated, USA

In this paper, the microstrip patch antenna and RF devices has been designed, fabricated and characterized on the multilayered alumina ribbon ceramic (RC) substrate for 5G wireless communication. The 40um alumina RC substrate with a relative permittivity ϵ_r of 9.8 and a loss tangent $\tan\delta$ of 0.0001 is fabricated by Corning's proprietary process of continuously sintered ceramic (CSC) process, which produces fine grain (~1u), high density (<0.5% porosity), high purity alumina (>99.9%) as well as ultrathin and availability in long length form factor (up to 100m). The transmission lines with three different line lengths and the ring resonator are designed on the single layer of the 40um alumina RC substrate to characterize the material properties and transmission loss at 28GHz. The microstrip patch antenna for 5G is also designed on the laminated three alumina substrates by using Cu-to-Cu bonding technique after metalizing each layer. This work demonstrates process feasibility and a huge potential of using ultra-thin and pure ribbon ceramic materials for high performance antenna/RF devices for 5G, mmWave even THz applications since the key substrate material can be designed and fabricated by the desired device performance through Corning's CSC process.

11:45 AM

(EMA-S12-005-2020) RF Modeling of Tunable Varactors with Thin Oxide Electrodes (Invited)

H. Maune¹; D. Walk¹; P. Komissinskiy²; L. Alf²; R. Jakoby¹

1. Technische Universität Darmstadt, Institute for Microwave Engineering and Photonics, Germany
2. Technische Universität Darmstadt, Advanced Thin Film Technology, Germany

Frequency tuning can be introduced into RF frontends by deploying tunable capacitors (varactors). Recent research proved the feasibility of conducting oxides as electrode materials for BST-based thin-film varactors in metal-insulator-metal (MIM) configuration. Dielectric characterization and modeling play an essential

role for developing new technologies and materials for RF systems. On the physical side, test structures are available that only require patterning of the top layer and allow a fast characterization. On the modeling side, time-consuming 3D EM simulations are necessary to extract the corresponding material properties. While analytic/schematic modeling would be fast, no accurate models that closely fit the dispersive characteristic are available up to now. Thin electrodes with thickness below the skin depth as used in the novel all-oxide thin-film varactors pose a challenge for common models. The talk features all steps from material selection and processing, RF characterization up to modeling of layer stack and component. We present a novel analytic model that splits the electrode's contribution into two parts and adds a parallel substrate impedance. Contrary to the common model, it is consistent over varying thickness of the dielectric and electrode, electrode conductivity and dielectric properties. Analysis shows that the root mean squared error (RMSE) can be decreased by orders with the new model.

12:00 PM

(EMA-S12-006-2020) Dielectric Characterization of Materials for Copper Clad Laminates at Microwave Frequencies

C. Grabowski¹

1. SABIC, USA

5G wireless technology is driving development of improved copper clad laminates (CCLs) for next-generation printed circuit boards and antennas that transmit data faster with lower signal loss at millimeter-wave frequencies. Optimizing the dielectric behavior of materials that comprise the laminate – typically consisting of a reinforced polymer resin mixed with inorganic fillers – is critical in helping us reach the needed performance targets. Techniques for measuring dielectric permittivity and loss tangent at microwave frequencies shall be explored in this talk. The equipment, measurement protocol, and sample form factors required for dielectric characterization are topic areas for discussion.

12:15 PM

(EMA-S12-007-2020) Realization and properties of the first nitride perovskite LaWN₃

K. Talley¹; R. Sherbondy²; J. Mangum¹; C. Perkins³; R. Woods-Robinson³; B. Gorman¹; A. Mehta⁴; G. L. Brennecke¹; A. Zakutayev²

1. Colorado School of Mines, USA
2. National Renewable Energy Laboratory, USA
3. University of California, Berkeley, USA
4. SLAC National Accelerator Laboratory, USA

The perovskite structure is a favorite playground for electroceramists across a wide variety of applications, and recent developments on hybrid metallorganic perovskite photovoltaics has renewed interest in expanding the chemical space of this flexible and multifunctional crystal structure. Development of highly engineerable nitride perovskites could potentially simplify integration of a number of functional (e.g., ferroelectric, piezoelectric, and more) properties directly with nitride semiconductors for a variety of integrated applications. In part because of the high valence cations needed to satisfy the high valency of nitrogen, and in forming nitride perovskite materials, and in part because of the challenge of limiting oxygen impurities, there are currently no literature reports of experimentally-realized pure nitride perovskites. Computational predictions of energetically favorable nitride perovskites, however, have been reported and DFT+LDA methods suggest that the lowest energy state of LaWN₃ is a non-centrosymmetric R3c type distorted perovskite structure with a spontaneous polarization of approximately 60μC/cm². Here we report the experimental confirmation of oxygen-free LaWN₃ as a perovskite using multiple fabrication approaches. Synchrotron scattering measurements accompanied by a substantial piezoelectric response confirm the R3c point group.

Theory, Modeling, and New Measurement Modalities in 5G

Room: Cypress C

Session Chairs: Geoff Brennecke, Colorado School of Mines;
Nate Orloff, NIST

2:00 PM

(EMA-S12-008-2020) A Transmission-Line Integrated Terahertz Source for Large-Amplitude Optoelectric Signal Synthesis (Invited)

K. Smith^{*1}; A. D. Feldman²; N. Orloff³; C. Long¹; N. Jungwirth¹; B. Bosworth¹

1. National Institute of Standards and Technology, RF Technology Division, USA
2. National Institute of Standards and Technology, USA
3. NIST, Communications Technology Laboratory, USA

In the telecommunications industry a range of frequencies are used to meet consumer and industrial needs, though it remains a challenge to bridge the gap from 100 GHz to 1 THz. The development of next-generation wireless communication, computer processing, and other high-speed technologies is underway at commercial semiconductor foundries, but the lack of proper diagnostic signals force manufacturers to design equipment through a time intensive, and costly, trial-and-error process. An optical-based network analysis approach utilizing continuous-wave (CW) terahertz photomixing devices fabricated on electro-optic substrates will allow for high bandwidth, tunability, and fine frequency resolution. Here, we demonstrate an on-chip, transmission line integrated photomixer for optical-to-electrical conversion up to 1 THz. Success of optical to electrical conversion up to 1 THz relies balancing material properties by optimization of tunable photocarrier lifetimes, reduced dark current, and improved internal quantum efficiency.

2:30 PM

(EMA-S12-009-2020) Frequency-Comb-Based Detection for Broadband Millimeter-Wave/Terahertz Sensing (Invited)

B. Jamali¹; A. Babakhani^{*1}

1. University of California, Los Angeles, USA

Broadband coherent detection in millimeter-wave and terahertz frequencies paves the way for novel sensing applications that stretch beyond 5G systems. Miniaturizing a broadband coherent detector on a CMOS integrated circuit can realize such applications with a low-cost, compact solution. In this work, we introduce a fully integrated coherent detector which uses a broadband frequency comb as a reference to detect mm-wave and sub-THz signals. High-speed current switches generate ultra-short pulses locked to an external clock rate, which sets the spacing of the comb in frequency domain. The frequency comb drives a passive field-effect transistor mixer to down-convert signals captured by an on-chip elliptical antenna. This detector circuit is fabricated in a standard 65-nm CMOS technology and it occupies a total die area of 0.56 mm². The system is capable of detecting any arbitrary spectrum from 50 to 280 GHz with a resolution of 2 Hz. Tunability of the frequency comb spacing allows us to scan a wide range of frequencies with a desired resolution. The detector circuit consumes a dc power of 34 mW, which makes it a low-power solution in comparison with conventional mm-wave/THz systems. Broadband spectroscopy and sensing systems can utilize this detector as it extracts precise frequency information of received signals.

3:00 PM

(EMA-S12-010-2020) Towards ultrafast control of dielectric response through optical phonon excitation (Invited)

G. Khalsa^{*1}; N. Benedek¹; J. Moses¹

1. Cornell University, USA

The development of short duration, intense, optical pulses in the mid- and far-infrared have created an opportunity to explore materials physics in a regime often thought to be uninteresting because of large optical absorption by infrared active (IR) phonons. The direct excitation of IR phonons has led to intriguing experimental discoveries in correlated materials ranging from the enhancement of superconductivity, to controlled ultrafast alteration of magnetism to transient switching of ferroelectric domains. Large amplitude IR phonons couple to Raman active phonons through nonlinear force-constants and the nonlinear polarizability. These two channels provide new flexibility for ultrafast control of crystalline symmetry and dielectric response, but also present new challenges due to the complexity of multi-phonon processes. In this talk, I will discuss our theoretical efforts towards ultrafast control of dielectric properties of materials over a broad frequency range including the telecommunication window.

3:15 PM

(EMA-S12-011-2020) Circuit Design at Extreme: Pushing the Limits of Silicon (Invited)

E. Afshari^{*1}; M. Tavakoli Taba¹; L. Chen¹

1. University of Michigan, USA

There is an increasing interest in low cost THz systems for medical imaging, spectroscopy, and high data rate communication. Recent results in the lower THz frequencies (<1THz) suggests that standard CMOS/BiCMOS processes can compete with compound semiconductors for some applications. In this talk, we present a few “real” applications for the CMOS THz systems as well as a few “fake” ones. Next, we discuss major challenges in realizing these systems in CMOS. Moreover, we show several novel methods to overcome these challenges to generate high powers with relatively low noise using oscillators, amplifiers, and frequency multipliers. Finally, we show how we can realize more complicated systems such as 2-D phased arrays and coherent imaging systems in silicon.

3:30 PM

(EMA-S12-012-2020) The ever-increasing importance of data science and data engineering for rapidly evolving technology: Why to learn programing + how to get started

A. Fox^{*1}

1. Qorvo Inc., USA

Up and coming technologies like 5G require a multitude of material and physical properties to be controlled to much tighter tolerances than most similar current technology. Classic methods of data management and processing (e.g. spreadsheets and file structures) while somewhat effective are inefficient, lead to lost data, and make it difficult, if not impossible, to look at all possible correlations or make decisions on the fly. All of which makes it difficult to meet the required tighter tolerances. Decisions about a layer you are about to process depend on the rest of the stack (its history and material properties) and experience with similar devices. To make these decisions you need all the data at your fingertips and you need to know how to process it. Traditionally this was a lot of repeated work in spreadsheets, but you can automate most of that process. While you automate, you can also perform data exploration or even apply your favorite buzz word algorithm (e.g. Machine Learning) to help find out how to improve the process. The industry is going to need more Materials Engineers with Data Science abilities. In this talk, I will dig into why you should learn to program, give some general examples, and offer suggestions of how to get started.

3:45 PM

(EMA-S12-013-2020) Bridging the Gap between Electromagnetic and Quantum Transport in the Analysis of Nanomaterials-based Devices (Invited)L. Pierantoni*¹

1. Università Politecnica della Marche, Dipartimento Ingegneria dell'Informazione, Italy

Nano-structured materials include atomic thick (1D-2D) materials as carbon nanotubes, graphene, beyond graphene, but also other atomically smooth surfaces as ferro-electric (e.g. HfO₂), ferro-magnetic materials. Today, most product development for these materials is hindered not by technology limitations but because of the limited reach of modeling and design tools that should instead encompass a wide range of spatial and time scales, with accuracy compared to that of available experimental and process data, and within affordable computational resources. Another limit for the design of some classes of 2D artificial material is less evident: the need for a theoretical model at “intermediate” scales for the conception of functionalized materials, that could be seamlessly integrated into the computational framework for subsequent optimization. In order to link quantum and electromagnetic models, we developed a computational platform made of a cascade of programs that perform simulations bridging from discrete, atomistic (few-to-hundred nm) level to continuum, meso-to-nano-scale level (micron to mm) level.

4:30 PM

(EMA-S12-014-2020) Computational studies of transitional behavior in dielectrics at mesoscale (Invited)J. Mangeri¹; D. Zhu²; K. Co³; P. Alpay³; A. Hagerstrom⁴; N. Orloff¹; S. Nakhmanson*³

1. Institute of Physics, Czech Academy of Sciences, Dielectrics, Czechia
2. Wuhan University, School of Civil Engineering, China
3. University of Connecticut, Materials Science and Engineering, USA
4. NIST, Communications Technology Laboratory, USA

Ferret is an open-source highly scalable real-space finite-element-method (FEM) based code for simulating transitional behavior of material systems with coupled physical properties at mesoscale. This code is built on MOOSE, Multiphysics Object Oriented Simulation Environment, which allows efficient solving of coupled-physics problems, has a proven record of efficient scaling of execution on up to 10K nodes, and is easily extendable to include new physical models. This approach allows treatment of structures possessing complicated morphology and evaluation of property dependencies on the system shape, size, microstructure and applied boundary conditions. In this presentation we provide an overview of Ferret's technical features and highlight its computational capabilities using a variety of examples. These applications include an investigation of transitional behavior in ferroelectric-dielectric composites and studies of the relaxation dynamics and dielectric tunability in the Ba_xSr_{1-x}TiO₃ perovskite ferroelectric, which has already seen integration into prototype devices for 5G electronics. For the latter case, possible effects of changing Sr concentration, inhomogeneous stress fields and polar domain topologies on the dielectric response and losses are also probed.

5:00 PM

(EMA-S12-015-2020) Using first principles methods to understand and optimize the properties of microwave ceramic dielectrics for 5G systems (Invited)N. Newman*¹; J. Gonzales¹; C. Muhich²

1. Arizona State University, Materials Program, USA
2. Arizona State University, Chemical Engineering, USA

The development of 5G technology requires low-loss temperature-compensated ceramics with enhanced dielectric constants. Despite their practical importance, a lack of a strong fundamental

understanding of the mechanisms has prevented the development of accurate quantitative predictions of the microwave dielectric properties. I will describe experimental and theoretical work that enables the field to gain a fundamental understanding of the mechanism(s) responsible for the microwave dielectric constant (ϵ_r), the loss tangent ($\tan \delta$) and the temperature coefficient of resonant frequency (τ_f). We will address the properties of commonly-used host compounds (e.g. Al₂O₃, BaZn_{1/3}Nb_{2/3}O₃, BaZn_{1/3}Ta_{2/3}O₃, SrIn_{1/2}Nb_{1/2}O₃, BaGd_{1/2}Nb_{1/2}O₃), as well as when doped with the most common impurities in commercial microwave dielectrics (e.g. Ni, Co, Mn, Zr). I will also describe how this understanding has allowed us to engineer switchable ultra-high Q dielectric microwave resonators and filters that be turned from a low-loss “on” state to a high-loss “off” state at small magnetic fields.

5:15 PM

(EMA-S12-016-2020) W-band dielectric property characterization of yttria-stabilized zirconia at high temperatureL. Enright*¹; M. Telmer²; M. Hilario³; A. E. Baros⁴; B. W. Hoff¹

1. University of Connecticut, Materials Science and Engineering, USA
2. Carnegie Mellon University, USA
3. University of Southern California, USA
4. Air Force Research Lab, USA

Yttria-stabilized zirconia (YSZ) has shown promise as a material for extreme environment electronic applications due to its high thermal stability, high temperature mechanical properties, and its electronic properties e.g. ion conduction. With rising prominence of W-band applications, materials are needed to optimize performance of W-band devices. This work explores the underlying mechanisms that lead to extraordinary properties in YSZ. Understanding of these mechanisms will enable the optimization of YSZ and other materials that might serve as candidates for W-band applications. As part of the present investigation, the dielectric properties YSZ samples were characterized at W-band frequencies (75 – 110 GHz) at temperatures ranging from 25°C to 800°C using free-space, focused beam methods.

S14: Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics**Materials by Design**

Room: Magnolia B/C

Session Chair: Mina Yoon, Oak Ridge National Laboratory

10:00 AM

(EMA-S14-001-2020) Modeling Bimetallic Nanoparticles: From Stability to Catalysis (Invited)G. Mpourmpakis*¹

1. University of Pittsburgh, Chemical Engineering, USA

Metal nanoparticles find tremendous applications in numerous and diverse areas, including medicine, catalysis, energy, and the environment. Despite these applications, the fundamentals of nanoparticle properties, such as stability and surface adsorption as a function of nanoparticle size, shape and metal composition are yet to be found. In this work, we blend first-principles calculations with computational modeling and machine learning to develop models able to capture thermodynamic stability, mixing properties and adsorption behavior of bimetallic nanoparticles of any morphology (size/shape) and metal composition. Our models are universal, rapid and able to capture a large number of computational and experimental data. Importantly, they take into consideration atomic level chemical bonding information on metal nanoparticles, revealing how different sites contribute to the overall property response on

bimetallic nanoparticles. Our developed models accelerate the discovery of nanomaterials by rapidly screening bimetallic nanoparticles with targeted application performance.

10:30 AM

(EMA-S14-002-2020) Modeling of Complex Inorganic Materials for Energy Applications with First Principles and Machine Learning Models (Invited)

N. Artrith*¹

1. Columbia University, Chemical Engineering, USA

Many commercially relevant materials have compositions with multiple chemical species and properties that are determined by complex structural features. This complexity makes them challenging to model directly with first principles methods. As an alternative, machine-learning techniques can be used to interpolate first principles calculations. Such machine-learning potentials (MLPs) enable linear-scaling atomistic simulations with an accuracy that is close to the reference method at a fraction of the computational cost. Here, I will give an overview of recent applications of MLPs based on artificial neural networks (ANNs) to the modeling of challenging materials classes, e.g., nanoalloys in solution, oxide nanoparticles, and amorphous materials. The original multi-species ANN potential formalism scales quadratically with the number of chemical species. This has previously prevented the modeling of compositions with more than a few elements. To overcome this limitation, we have recently developed an alternative mathematically simple and computationally efficient descriptor with a complexity that is independent of the number of chemical species. The new method has been implemented in our free and open source atomic energy network (aenet) package (<http://ann.atomistic.net>). This development creates new opportunities for the modeling of complex materials.

11:00 AM

(EMA-S14-003-2020) Prediction of Two-Dimensional Organic Topological Materials in Several Metal Organic Frameworks (Invited)

L. Zhang*¹; M. Yoon²

1. University of Tennessee, USA

2. Oak Ridge National Laboratory, USA

Two-dimensional topological materials, such as quantum spin/ anomalous Hall insulators (QSHI/QAHI), 2D Dirac/Weyl/node-line semimetals (2DSM/2DWSM/2DNSM), are a highly promising class of materials for spintronic devices and quantum computations. To date, the investigations of topological materials are mainly focused on inorganic systems. Compared to the inorganic materials, organic materials have potentially the advantages of low cost, easy fabrications, and mechanical flexibility. Here, we propose several 2D organic topological materials in three families of 2D metal (M) organic frameworks (MOF): $M_2(DCA)_3$ ($M = Cu, Au$), $M_2(C_2O_4)_3$ ($M = Re, Pt, Hg$), and M-1,3-BPyB ($M = Cu, Fe$). First-principles calculations show that $M_2(DCA)_3$ ($M = Cu, Au$) are intrinsic QSHI which have been synthesized in experiment, $Re_2(C_2O_4)_3$ is a room-temperature QAHI with the spin-orbit coupling gaps ~ 160 meV and Curie temperature ~ 380 K, $Pt_2(C_2O_4)_3$ is a 2DWSM with the in-plane magnetic moment, and Cu-1,3-BPyB is a 2DNSM. Based on the orbital and tight-binding model analysis, we also confirm their topological properties and explain the original of these properties. Our findings not only enrich the families of the topological materials, but also provide a new avenue to track these materials in the 2D MOF systems.

11:30 AM

(EMA-S14-004-2020) Anomalous Dirac Plasmons in 1D Electrides (Invited)

B. Huang*¹

1. Beijing Computational Science Research Center, China

Plasmon opens up the possibility to efficiently couple light and matter at sub-wavelength scales. In general, the plasmon frequency is dependent on carrier density. This dependency, however, renders fundamentally a weak plasmon intensity at low frequency, especially for Dirac plasmon (DP) widely studied in graphene. Here we demonstrate a new type of DP, excited by a Dirac nodal-surface state, which exhibits an anomalously density-independent frequency. Remarkably, we predict the realization of anomalous DP (ADP) in 1D electrides, such as Ba_3CrN_3 and Sr_3CrN_3 , by first-principles calculations. The ADPs in both systems have a density-independent frequency and high intensity, and their frequency can be tuned from terahertz to mid-infrared by changing the excitation direction. Furthermore, the intrinsic weak electron-phonon coupling of anionic electrons in electrides affords an added advantage of ultra-low phonon-assisted damping and hence a long lifetime of the ADPs. Our work paves the way to developing novel plasmonic and optoelectronic devices by combining topological physics with electride materials.

12:00 PM

(EMA-S14-005-2020) Defect Formation in Various Oxide Lattices by Re-Visiting of Madelung Lattice Energy and Lattice Site Potentials

M. Yoshimura*¹

1. National Cheng Kung University, Hi-GEM & PCGMR, Mater. Sci. & Eng., Taiwan

Point defect (Vacancy) formation is the most important key issue in many functional ceramics, particularly in SOFC, Li-Battery, Catalysis, etc. That defect formation should be discussed by thermodynamics using Free Energy (G) of such defects, but unfortunately all of them have not been available even now. However, Lattice energy: U (Enthalpy: H at 0K) can be easily available and calculable, then it would be 90-95% of G. Total Lattice energy can be considered by Sub-lattice energies. Which can be considered every site potential of Cation and Anion sites: i.e. Φ_A , Φ_B and Φ_O in Perovskite ABO_3 . A vacancy (point defect) would form in a shallower potential site but would be difficult in a deeper potential site, therefore, A-site defect might be easier than B-site because Φ_B is always deeper than Φ_A in all Perovskite lattices. Based upon Lattice site potentials in various oxides, one can see that Oxygen defect(s) would form in shallow potential site(s) in the lattice: i.e. Oxygen defects would form more easily in $LaGaO_3$, CeO_2 , etc. Exceed a critical value (say 1.65 \AA^{-1}) Oxygen defects would not form but rather edge sharing structure like shear structure by collapsing the defects would form: i.e. tungsten bronze and/or Magneli phases. Of course recent "first principle calculation" will more perspective but take more time and cost.

12:15 PM

(EMA-S14-006-2020) Lattice and Valence Stability in Perovskite Oxide Lattice by Re-Visiting of Madelung Lattice Energy and Lattice Site Potentials

M. Yoshimura*¹

1. National Cheng Kung University, Hi-GEM & PCGMR, Mater. Sci. & Eng., Taiwan

So many compounds with Perovskite: ABO_3 and/or its related structures have been found and used in various functional areas, however the reason why they would take Perovskite structure(s) have not well been understood. Ion packing model like Tolerance Factor, Goldschmidt (1923) has still been used. Stability should be

discussed by thermodynamics using Free Energy(G) but unfortunately all of them have not been available even now. However, Lattice energy:U (Enthalpy:H at 0K) can be easily available, then it would be 90-95% of G. The calculated results have clearly showed that Perovskite lattices have Larger U than the summation of U for their components: AO+BO₂, A₂O₃+B₂O₃, etc. Furthermore, when one has considered every site potential: Φ_A , Φ_B and Φ_O , A-site prefers shallower potential, B-site prefers deeper potential and O-site is arranged by A-site and B-site, therefore, low valence ion(s) would occupy A-site while high valence ion(s) occupy B-site. Sometimes un-conventional higher valence ions, like Co³⁺, Ni³⁺, Fe⁴⁺ might be stabilized by high Φ_B compensating their ionization potential(s). Since Valence stability of ions is mostly(>90%) function of lattice site potential nevertheless the coordination and crystal structures, Entropy term:ST has minor (<10%) effect. Recent "first principle calculation" will more perspective but take more time and cost.

12:30 PM

(EMA-S14-007-2020) Genetic algorithm for prediction of surface phase diagrams of 2D films on substrate

V. Kolluru^{*1}; P. Ghanekar²; J. Greeley²; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA
2. Purdue University, Department of Chemical Engineering, USA

Substrates influence the stability and properties of 2D materials. It is important to understand the interactions of the 2D material when comes in contact with a substrate. We search for stable surface configurations using a modified evolutionary algorithm. We predict the surface phase diagram of different 2D films on a substrate by using an objective function determined by chemical potentials of species in the 2D layer. The algorithm starts with user provided or randomly generated 2D films and performs genetic operations within the 2D layer to create new structures. We lattice match the created 2D layer with given substrate limited by maximum allowed strain and area. The interface structures thus created are evaluated using VASP or LAMMPS. We initially test the algorithm on Si (100) surface and successfully found the stable dimer configuration. The search of stable oxide structures on Pd (111) surface is currently ongoing. We found ordered single layer structures at compositions ranging from pure Pd to PdO₂. We vary the oxygen chemical potentials and report a surface phase diagram within the composition range. The results will be compared with the experimental observations. This algorithm helps to discover stable 2D phases on substrates thereby accelerating experimental synthesis. It also helps as a tool to theoretically investigate the experimental findings.

Predictive Modeling/Novel Phenomena

Room: Magnolia B/C

Session Chair: Aloysius Soon, Yonsei University

2:00 PM

(EMA-S14-008-2020) Ceramic lithium and sodium ion conductors for solid state batteries: From bulk structure to functional device (Invited)

D. Fattakhova-Rohlfing^{*1}

1. Forschungszentrum Juelich, Institute of Energy and Climate Research IEK-1, Germany

Solid-state batteries are intensively investigated as a possible energy storage technology able to improve safety and increase energy density of electrochemical energy storage devices. An important requirement for the development of efficient batteries is a sufficiently high ionic conductivity of the electrolyte layers, necessitating the search for novel solid electrolyte systems with enhanced conductivity. Among different solid electrolyte classes, oxide and phosphate-based solid ionic conductors for lithium and sodium such

as garnet type or NASICON-type ceramics show sufficient ionic conductivities in the range of mS/cm at room temperature. A great challenge however facing ceramic electrolytes is a great impact of synthesis and processing conditions on the total ionic conductivity in addition to the bulk crystal structure. Furthermore, the practical realization of solid batteries requires integration of the solid ionic conductors in a full device, raising the issues of material compatibility and formation of possible interphases influencing the total cell resistance. I will discuss the fundamental and application-related properties of oxide- and phosphate-type ceramic electrolytes such as structure, processing- and morphology-dependent conductivity, which provides a basis for the development of efficient solid-state electrochemical storage devices.

2:30 PM

(EMA-S14-009-2020) Ceramic Proton Conductors based on Perovskites for Energy and Environmental Applications (Invited)

M. E. Ivanova^{*1}; N. H. Menzler¹; O. Guillon¹

1. Forschungszentrum Jülich GmbH, IEK-1, Germany

The global effort for reaching highly efficient CO₂-neutral energy supply requires innovative technological solutions based on high performance materials. Ceramic proton conductors (PC) with tailored properties gain increasing scientific and industrial interest due to their multifaceted low temperature applications. Reversible PC electrolysis/fuel cell devices can convert and store electrical surplus from renewables into H₂ or NH₃, which is then used as fuel when power generation is required. Renewably electrified PC co-electrolysers utilize CO₂ emissions electrochemically to i.e. CH₄, CH₃OH, or Syngas, while natural gas fuelled PC cells can co-generate electricity and valuable chemicals, e.g. olefins or aromatics (i.e. C₂H₄, C₂H₂, or C₆H₆). Such concepts of ceramic PC integration offer significant process intensification resulting in higher overall energy efficiency, products selectivity and yields. The present talk will give an overview on different functional and utilization aspects of selected proton conductors based on perovskites (e.g. BaZr_{1-x}(Ce,Y)_xO_{3-δ}) and ceramic composites (BaZr_{1-x}(Ce,M)_xO_{3-δ}:Ce_{1-x}M_xO_{2-δ}) in the light of achieving green and sustainable economy.

3:00 PM

(EMA-S14-010-2020) Role of the MA cation on fundamental properties of hybrid halide perovskites (Invited)

J. Lee^{*1}

1. Korea Institute of Science and Technology, Republic of Korea

Hybrid halide perovskites have been under intense investigation due to their high-power conversion efficiencies and low cost for solar cell applications. To further improve the efficiency of the perovskite solar cell, we need to find and understand control parameters for tuning fundamental properties of hybrid halide perovskites. Herein we investigate the effect of methylammonium (MA) on the electronic structure, mechanical properties, and thermodynamic stability of hybrid halide perovskites using van der Waals (vdW)-corrected density functional theory (DFT) calculations. According to our calculations, hydrogen bonding between an organic MA cation and the halide frame induces the octahedral tilting which affects the optical band gap and carrier effective masses. In addition, we show that the MA cation improves the material's resistance to deformation. For example, the orientationally-averaged Young's modulus of orthorhombic MAPbI₃ increases by about 19% compared to the equivalent inorganic series of structures. We further show that the MA cation is mainly responsible for the pressure-induced phase transition in MAPbI₃. Taken together, these results can help guide the optimization of the fundamental properties of perovskite-based solar cell materials.

4:00 PM

(EMA-S14-011-2020) Kinetic-controlled solid-phase bulk heteroepitaxy of formamidinium lead halide perovskite (Invited)

J. Lee^{*1}; S. Tan⁴; T. Han⁶; L. Zhang⁵; C. Park²; M. Yoon³; Y. Yang⁴

1. SungKyunKwan University, SKKU Advanced Institute of Nanotechnology (SAINT) and Department of Nanoengineering, Republic of Korea
2. Oak Ridge National Laboratory, Center for Nanophase Materials Science, USA
3. Oak Ridge National Laboratory, USA
4. University of California, Los Angeles, Department of Materials Science and Engineering and California NanoSystems Institute, USA
5. University of Tennessee, Knoxville, Department of Physics and Astronomy, USA
6. Hanyang University, Division of Materials Science and Engineering, Republic of Korea

Epitaxial growth is one of the most powerful ways to fabricate semiconducting thin films with low defect density and a desired orientation. However, the conventional epitaxy of semiconductor films requires a compatible single crystalline substrate and precisely controlled growth conditions, which limit the price competitiveness and versatility of the process. Here, we demonstrate substrate-tolerant bulk heteroepitaxy (BHE) of high-quality formamidinium-lead-tri-iodide (FAPbI₃) perovskite thin films with controlled crystal growth kinetics. The first-principles calculations revealed a new mechanism involved in the growth kinetics associated with a synergistic effect between strain and entropy. The slow heteroepitaxial crystal growth enabled 16-fold enlarged perovskite crystals with a reduced defect density and strong preferred orientation. Our BHE is readily applicable to various substrates used for devices. The proof-of-concept solar cell and light-emitting diode devices based on the BHE-FAPbI₃ showed efficiencies and stabilities superior to those of devices fabricated without BHE.

4:30 PM

(EMA-S14-012-2020) Computational Prediction and Experimental Realization of New Nitride Materials

S. Bauers¹; K. Heinselman¹; E. Arca¹; W. Sun³; C. Bartel²; A. Holder²; S. Lany¹; G. Ceder³; A. Zakutayev^{*1}

1. National Renewable Energy Laboratory, USA
2. University of Colorado, USA
3. University of California, USA

Agile design of new electronic materials is one of the most important directions in materials research. Certain materials chemistries, such as oxides, have been extensively explored in the past. Other related chemistries, including nitrides, have been barely looked at. This presentation will describe computationally driven experimental discovery of new nitride materials, focusing on experimental synthesis and characterization, following computational predictions and machine learning. The data mining, first-principles calculations, and machine learning analysis indicated predicted 244 new stable ternary nitride compounds. Experimental synthesis using high-throughput combinatorial methods realized 7 of these compounds, such as Mg-TM-N (TM = Nb, Ti, Zr, Hf) and Zn-M-N (M = Sb, Mo, W). The Mg-TM-N ternary rocksalts are semiconductors with 1.8-2.1 eV optical absorption onsets and large dielectric constants. The Zn-Sb-N and Mg-Sb-N wurtzites are the first reported Sb-containing nitrides, with Sb in unusually high 5+ oxidation state.

4:45 PM

(EMA-S14-013-2020) Energetics and electronic properties of dopants, defects, and defect complexes in 2D transition metal dichalcogenides from first-principles

A. Z. Tan^{*1}; C. Freysoldt²; A. Kozhakhmetov³; J. A. Robinson³; R. G. Hennig¹

1. University of Florida, USA
2. Max-Planck-Institut für Eisenforschung GmbH, Germany
3. The Pennsylvania State University, USA

Two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDCs) have attracted extensive research interests for potential applications in optoelectronics, spintronics, photovoltaics, and catalysis. To harness the potential of 2D semiconductors for electronic devices requires a better understanding of impurities, defects, and dopants and how they control the carrier concentration, character, and mobility in 2D materials. Accurate determination of defect formation energies and charge transition levels enables us to predict their effect on the electronic properties and how they respond to changes in synthesis and processing. We collaborate with experimental groups at the 2D Crystal Consortium (2DCC) to identify defects and dopants of interest in technologically relevant TMDCs such as MoS₂ and WSe₂ and perform density functional theory calculations to accurately compute their formation energies, charge transition levels, and electronic structures. We identify dopants which can form defect complexes with intrinsic defects such as vacancies, modifying the electronic properties of the individual defects. We are also developing a Python-based workflow to facilitate efficient high-throughput calculations of charged point defects in a wide range of 2D materials.

5:00 PM

(EMA-S14-014-2020) Polymorphic expressions in epitaxially strained alkali-metal niobates

W. Hwang^{*1}; S. Yoon¹; A. Soon¹

1. Yonsei university, Republic of Korea

There has been an increased interest in piezophotonic materials – the coupling of piezoelectric polarization and semiconductor optical properties in non-centrosymmetric polar compounds. The perovskite-structured alkali metal niobates (namely, KNbO₃ and NaNbO₃) are attractive and potential substitutes for lead-based piezoelectrics given that they are non-toxic and possess attractive piezoelectric properties. However, despite their excellent piezoelectric properties, the large energy band gap (>3 eV) in these niobates poses a critical hurdle for visible-light emission applications. In this work, we perform first-principles density-functional theory (DFT) calculations to examine how polymorphic expressions in both KNbO₃ and NaNbO₃ can influence their structural, thermodynamic, electronic, and piezoelectric properties under epitaxial strain. Our theoretical results provide the structure-property relationships in these perovskite-structured alkali metal niobates and the accompanied tunable band-gap energies, especially under the influence of epitaxial strain, may lend support in the designing new materials for the next-generation piezophotonic applications.

5:15 PM

(EMA-S14-015-2020) Mechanical Control of Topological Properties: A First Principles Analysis of Bi₂Se₃, Bi₂Te₃, and As₂Te₃

T. K. Reid^{*1}; P. Alpay¹; A. Balatsky²; S. Nayak¹

1. University of Connecticut, Materials Science and Engineering and Institute of Materials Science, USA
2. KTH Royal Institute of Technology, Nordita, Sweden

We present the results of two related computational studies on first-principles modeling of binary layered topological insulators (TIs). First, we employed density functional theory (DFT) to perform a systematic analysis of the response of the electronic band structure of Bi₂Se₃ and Bi₂Te₃ to geometric optimization,

simultaneously varying the thickness of our slab models and the exchange-correlation functionals (XCF). After comprehensively searching the computational space, we conclude that the GGA+vdW functional is best suited for computational studies of this class of TIs. Further, we determine that electronic properties measured from models constructed with experimental lattice parameters (ELP) will likely be accurate. In a second study, we use DFT to study the response of the electronic band structure of As_2Te_3 and Bi_2Se_3 to biaxial strain. We use GGA+vdW as the XCF and ELP as the starting structure for both materials. In increments of 1% along in-plane, we adjust the lattice parameters of slabs of both materials from -4% to 4% of the original structure. We demonstrate closure of the bandgap in As_2Te_3 , a fundamental characteristic of TIs, under negative strain, whereas there is an opening in the bandgap in Bi_2Se_3 under positive strain. The results of these studies are important for the development of mechanically controlled topological and trivial insulator switches.

Poster Session

Room: Orange C/D

5:30 PM

(EMA-SP001-2020) Improving the electrical and ferroelectric properties of lead iron niobate by decreasing calcination temperature

N. Bartek^{*1}; S. V. Vladimir¹; D. C. Lupascu¹

1. University of Duisburg-Essen, Institute for Materials Science, Germany

Lead iron niobate, $\text{Pb}(\text{Fe}_{0.5}\text{Nb}_{0.5})\text{O}_3$ (PFN), is a multiferroic material, in which ferroelectric and antiferromagnetic order coexist and dielectric and magnetic properties have been studied in PFN ceramics a lot. Although there are many synthesis routes for PFN, solid state is the simplest one, but to synthesize a pure perovskite phase a high calcination temperature from 850 °C is needed. Calcinating at such high temperatures results in lead loss, which influences the electrical properties a lot. At the same time, good electric insulation is necessary for achieving of sizable magnetoelectric effect. We focused on investigation of the changes in electrical behavior by decreasing the calcination temperature. Phase characterization was done using x-ray diffraction, electric properties were studied by dielectric spectroscopy, leakage current, and polarization versus electric field measurements. We found out, that after sintering over 1000 °C a pure perovskite phase can be achieved, even when it was not formed after calcination. Because of this the calcination temperature can be decreased and therefore the electrical properties got enhanced, namely the leakage current got reduced massively. Besides, dielectric permittivity ϵ increases from around 20.000 to 90.000 and P_{max} also increases from 8.14 to 13.69 $\mu\text{C}/\text{cm}^2$ at 15 kV/cm at the same sintering temperature.

(EMA-SP002-2020) Oxide Ion Conduction Mechanisms in Sodium Bismuth Titanate ($\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$)

C. M. Culbertson^{*1}; R. McQuade²; A. Paterson³; M. Lucero⁴; M. Dolgos⁵; Z. Feng⁶; D. Cann²

1. Oregon State University, Chemistry, USA
2. Oregon State University, School of Mechanical, Industrial, and Manufacturing Engineering, USA
3. University of Calgary, Canada
4. Oregon State University, Chemical Engineering, USA
5. University of Calgary, Chemistry, Canada
6. Oregon State University, School of Chemical, Biological, and Environmental Engineering, USA

Recent research has shown ionic conduction in sodium bismuth titanate [$\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$, (NBT)] based materials and the goal of this work is to develop a fundamental understanding of the dominant mechanisms that underpin this phenomenon. To accomplish this, a range of stoichiometric, non-stoichiometric and doped samples have been synthesized via solid state synthesis. To investigate the structure,

data on high resolution synchrotron diffraction, X-ray total scattering, and X-ray absorption spectroscopy have been collected. From the high resolution synchrotron diffraction data there are several clear phase transitions observed. At room temperature the structure of all samples is monoclinic Cc, around 400 C the structure is fully tetragonal P4bm, then at 500 C and above the structure is cubic Pm-3m. The local structure also shows a dramatic change in the first bismuth-bismuth coordination sphere, although the data is still to be analyzed. The physical properties measured thus far are the dielectric permittivity and loss that show that the conductivity can drastically be increased with bismuth deficiency and magnesium doping. Using these techniques, the structure and corresponding properties will be correlated to determine the charge carrier type and to identify average or local structural distortions that enable the observed high levels of oxygen conductivity.

(EMA-P003-2020) Growth of Silicon Nanowires on Silicon wafer for Improving Optical and Photovoltaic Properties

D. K. Shah¹; H. Lee¹; Y. Son¹; M. Akhtar¹; O. Yang¹; C. Kim^{*1}

1. Chonbuk National University, Semiconductor and Chemical Engineering, Republic of Korea

In this work, we report on the development of crystalline Si solar cells without using the AR layer. The Si wafer was textured by growing nanowires like nanostructures via wet controlled etching method and directly used for the fabrication of Si solar cell without AR. The nanowires on Si wafer were optimized in terms of sizes, lengths, and densities by changing the etching conditions. Well-defined and aligned wires like structures were achieved when the etching time was 20 to 30 min. The prepared Si nanowires displayed the minimum reflectance ~1.64% at 850 nm with the average reflectance of ~2.25% in the wavelength range from 400-1000 nm. The nanowires Si wafer based solar cells achieved the comparable power conversion efficiency in comparison with c-Si solar cells with SiN_x AR layer. From this study, it is confirmed that the controlled wet etching method is an easy, facile method for preparation of nanostructured like wires on Si wafer with low reflectance in the whole visible region, which has greater prospects in developing c-Si solar cells without AR layer at low cost.

(EMA-SP004-2020) Coupling of Electrochemical and Mechanical Properties in MoS_2 Electrodes

J. Johnson^{*1}; A. Mann¹

1. Rutgers University, Materials Science and Engineering, USA

To resolve the intermittency problem inherent to renewable energy sources like solar and wind, a high capacity energy storage device is needed. Metallic molybdenum disulfide (1T MoS_2) has been shown to be a high capacitance electrode material, applicable in lithium ion batteries. Computational and experimental research has also shown monolayer sheets of MoS_2 to be highly flexible with a Young's modulus comparable to steel, mechanical properties that are especially advantageous for long battery life. However, the application of 1T MoS_2 in macroscale devices requires a mechanical understanding that incorporates the interlayer interactions in restacked films. Here we show a method for measuring the electrochemical performance of macroscale 1T MoS_2 films under applied tensile strain to better analyze the coupling between electrochemical and mechanical properties. Our preliminary results indicate strain engineering enhances the rate capability and peak current values, possibly due to increased conductivity and widened diffusion paths. Our work demonstrates a simple method for tuning electrochemical properties and can be used to probe the coupling between mechanics and electrochemistry in other 2D materials.

*Denotes Presenter

(EMA-P005-2020) Electrical conductivity of synthesized diamonds in corrections with fractal nature analysis

S. Veljkovic²; V. Mitic^{*1}; G. Lazovic³; V. Paunovic²; M. Mohr⁴; H. Fecht⁴

1. Institute of Technical Sciences of SASA/University of Nis, Faculty of Electronic Engineering, Serbia
2. University of Nis, Faculty of Electronic Engineering, Serbia
3. University of Belgrade, Faculty of Mechanical Engineering, Serbia
4. Institute of Functional Nanosystems FNS, Ulm University, Germany

Polycrystalline diamonds are innovative materials and the phenomena of electrical conductivity is intensively researched. These materials, which have good mechanical and electrical properties, are very interesting for MEMS since there is a need to apply MEMS in both sensitive and harsh conditions. The electrical conductivity of ultra-nanocrystalline diamond films can range from 10^{-4} to 300 S/cm. The structural properties of high conductivity UNCD have been specifically investigated to determine its origin, which exhibits n-type conductivity at room temperature. In these tests, it was observed that there was a considerable amount of nano-graphite between the grains of diamond crystals. The structural properties of sp^2 carbon bonds and specific conductivity are observed. Thus, the specific conductivity is primarily influenced by the structural properties of the grain boundary. The very low activation energies (meV) of sp^2 hybridized carbon bonds explain the conductivity of these films at room temperature. As a result of the experiments carried out, it was clearly observed that with the increase of the mean size of the formed grains, which varied in the range from 3.5 nm to 12.5 nm, the specific electrical conductivity decreased intensively. The goal of this paper is to connect fractal approach with this phenomena of electrical conductivity and make correlation between them.

(EMA-P006-2020) Physical Characterization of α , β -FeOOH nanorod by controlling aspect ratio and silica coating

Y. Kim^{*1}

1. Korea Institute of Ceramic Engineering and Technology (KICET), Engineering Ceramic Center, Republic of Korea

We studied on the synthesis and characterization of the tunable α , β -FeOOH as a yellow pigment using controlling rod length and silica coating approach. The aspect ratio of α , β -FeOOH is related to their coloration and we evaluated the chromaticity by controlling the length/aspect ratio of α , β -FeOOH. In addition, the pH has a great influence on controlling the length of the yellow pigments. As a result, the aspect ratio of the α -FeOOH rod was controlled from 3.9 to 38.5. The β -FeOOH rod is easily tuned color change from redness to yellowness through various length and diameter. To enhance the properties of α , β -FeOOH pigment, we adopted silica coating approach. In particular, this study investigated the effect of silica shell on the density. We coated SiO_2 on α , β -FeOOH and tried to change the structure of the coating layer using a mild basic solution. We observed the change of shape by TEM (Transmission electron microscopy) analysis and selected the appropriate reaction time and compared the chromaticity according to the silica layer structure. In particular, it was confirmed that yolk-shell structure of yellow pigments had a median chromaticity value. Details of the coloration and phase structure of pigments were characterized by UV-vis, CIE Lab color parameter measurements, SEM (scanning electron microscopy) and XRD (powder X-ray diffraction).

(EMA-SP007-2020) Bio-wastes derived $Ca_2SiO_4:Sm^{3+}$ phosphors for solid state lighting applications

M. Kaur Chhina^{*1}; K. Singh¹

1. Thapar Institute of Engineering and Technology, School of Physics and Materials Science, India

Sm^{3+} activated Ca_2SiO_4 phosphors have been synthesized from bio-wastes (rice husk ash and egg shell powder), using solid state reaction method. Energy dispersive spectroscopy has been utilized for chemical analysis of the synthesized samples. X-ray diffraction

has been used as a tool to understand the influence of Sm^{3+} on the phase stability of monoclinic Ca_2SiO_4 phase. Fourier transform infrared spectroscopy provides information about the different structural units present in the synthesized phosphors. Optical properties of the phosphors have been studied using diffuse reflectance and photoluminescence spectroscopy which provided information about the band gap and emission spectra, respectively. Luminescence spectra consisted of typical bands of Sm^{3+} indicating that these phosphors can find use as cost effective substitutes of conventional solid state lighting sources. Additionally, the trace element oxides present in bio-wastes stabilized the monoclinic Ca_2SiO_4 phase. These inherent trace elements also resulted in emission in the visible region, hence can find use in optoelectronic applications.

(EMA-SP008-2020) W-Band Dielectric Constant Measurements of Slip-Cast Polycrystalline Alumina of Different Porosity by Varying Sintering Temperature

M. Hilario^{*1}

1. University of Southern California, USA

The complex dielectric constants of polycrystalline Alumina with varying porosity are reported at W-Band frequencies (75-110 GHz) for temperatures between 20-1000C using the free-space method. The Alumina samples were manufactured using conventional slip casting methods to vary porosity by sintering at temperatures between 1350-1600C. The density and open porosity is measured with the Archimedes method, and the distribution of the porosity and grain size distribution is measured by scanning electron microscopy. The effective dielectric constant is compared to dielectric mixing models including the Maxwell-Garnet effective medium approximations. The dielectric constant and loss parameters of the polycrystalline ceramic are also compared to previous temperature-dependent measurements of single crystal Alumina versus crystallographic orientation. Chemical and microstructural analyses are performed to identify mechanisms giving rise to millimeter-wave absorption and dielectric losses, and will include scanning electron microscopy, energy dispersive spectroscopy, x-ray diffraction, mass spectroscopy, DC conductivity measurements using a high temperature four-point probe, and temperature-dependent AC impedance (1Hz-10MHz) using a Solartron.

(EMA-SP009-2020) Photo-induced electrical behavior under gas incidence in 1at%Er³⁺ doped SnO₂ based thin films

D. H. de Oliveira Machado^{*1}; J. H. Dias da Silva¹; L. V. de Andrade Scalvi¹

1. Sao Paulo State University, Physis, Brazil

Tin oxide (SnO_2) is a transparent oxide semiconductor, with many applications, such as gas sensors, due to its sensitivity to many gases, including reducing and toxic gases. Gas sensors utilize changes in conductance to detecting a particular gas, which is improved when SnO_2 is doped or mixed with other metal oxides, depending on aimed gas type and operating conditions. This work presents results on isolated $SnO_2:Er$ evaporated thin films and forming the $GaAs/SnO_2:Er$ heterojunction. SnO_2 is deposited by resistive evaporation, where the powder for evaporation comes from the sol-gel route. Electrical measurements (photo-induced current decay) were performed after excitation with distinct monochromatic light sources: He-Ne laser (628nm) and InGaN LED (450nm), under influence of atmosphere rich in CO_2 or O_2 . Results for $SnO_2:Er$ (annealed at 1000°C), showed that after excitation with the InGaN LED at room temperature the decay rate (calculated from the maximum current) is 8.2% for O_2 and 21.6% for CO_2 , for a stabilization time of 50s in the sample current. Although the light energy is lower than the SnO_2 bandgap, it has high influence on sample excitation, ionizing efficiently intrabandgap states. Moreover, regardless of the LED excitation, the CO_2 gas induces electron capture from the sample, which is enhanced under light irradiance. Work supported by CNPq, CAPES and FAPESP (process 2016/12216-6)

(EMA-SP010-2020) Creating High Temperature Ferroelectrics by using Ternary Components with Limited SolubilityB. D. Hirt^{*1}; A. Sehirlioglu²; B. Kowalski³

1. Case Western Reserve University, Material Science and Engineering, USA
2. Case Western Reserve University, USA
3. NASA Glenn Research Center, USA

High temperature ferroelectrics are sought after for actuator applications ranging from drilling on the surface of Venus to fuel modulation in jet engines. In this study, we examined how the Curie temperature and other piezoelectric properties changed as we changed the end member of ternary systems. Our starting point was near the morphotopic phase boundary (MPB) between PbTiO_3 (PT) and BiScO_3 (BS) (62% and 38% respectively), and the third components in these ternary systems were suggested by machine learning. The third components added cannot be used as binary systems with PT due to inability to reach the morphotopic phase boundary composition as a result of limited solubility. The study will focus on PT-BS-BiCoFeO₃ (BCF) ternary component with varying BCF ((PT-BS)_{1-x}(BCF)_x) and a varying Co/Fe ratio ($\text{Bi}(\text{Co}_x\text{Fe}_{1-x})\text{O}_3$). The results will be compared to the binary PT-BS, as well as to piezoceramics in $(\text{BiScO}_3\text{-PbTiO}_3)_x\text{-}(\text{Bi}(\text{Zn}_x\text{Zr}_{1-x})\text{O}_3)_{1-x}$ (BS-PT-BZZ) ternary, that has been shown to have improved properties in comparison to the binary. As the BCF increased in the PT-BS-BCF system, the internal strain increased resulting in limited ability to pole the samples before breakdown. As the amount of cobalt concentration increased compared to iron in the PT-BS-BCF system, the internal strain decreased with improved ability to pole and the related changes in electromechanical properties.

(EMA-P011-2020) Effects of Gap Filling, Surface Roughness and Metal Work Function on Fast Rise Breakdown for Dielectric Filled Air GapJ. Sorenson^{*1}; C. Gomez¹; P. Yang¹

1. Sandia National Laboratories, Electrical, Optical and Nano-Materials, USA

Gas discharge provides unique capability for fast response, high current switching applications. The use of dielectric particles to enhance gas discharge to mitigate lightning hazards was first explored in the late 1960s because of the threat lightning posed to aerospace vehicles and solid-state electronics. This study investigates the gap filling, surface roughness and metal work function on the fast rise breakdown since these factors are important to field concentration and precursor breakdown. The average maximum breakdown voltage and average voltage ramp rate under the change of these parameters will be reported and analyzed based on underpinning mechanisms governing the gas discharge behavior. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(EMA-P012-2020) Fast-Rise Breakdown Mechanisms for a Varistor Filled Air GapC. Gomez¹; S. Andrews²; J. Sorenson¹; P. Yang^{*1}

1. Sandia National Laboratories, Electrical, Optical and Nano-Materials, USA
2. Sandia National Laboratories, Connectors and LACs, USA

Varistor materials used in surge protection applications possess a unique nonlinear voltage-current response to protect valuable assets by diverting unexpected high voltage surges to the ground. This investigation studies the breakdown behavior of a varistor filled air gap for lightning protection. Since lightning can strike several times and cause fire, the effects of temperature and pressure on the fast-rise breakdown are also investigated. Based on the characteristics of the varistor and the waveforms collected under these conditions, the breakdown mechanisms were analyzed. Special attention is paid to the intrinsic change in resistance, switching field, and breakdown

voltage. Results are paramount to the lightning protection devices' practical application. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(EMA-SP013-2020) The thermoelectric transport properties of polycrystalline SnSe-SnTe solid solutionsW. Jin^{*1}; J. Cho¹; K. Park¹; S. Muhammad³; J. Kim⁴; C. Park²

1. Seoul National University, Material Science and Engineering, Republic of Korea
2. Seoul National University, Republic of Korea
3. National University of Sciences and Technology, School of Material Science and Engineering, Pakistan
4. Korea Institute of Science and Technology, Republic of Korea

Tin selenide (SnSe) containing non-toxic and earth-abundant elements has been considered as a promising TE material. However, because of the poor mechanical properties and the difficulty of fabricating single crystal, many studies have been conducted to obtain polycrystalline SnSe having a high TE performance. The ZT values of polycrystalline SnSe are lower than the single crystal SnSe due to their relatively low electrical conductivity and high thermal conductivity. One potential way to optimize the TE performance of polycrystalline SnSe is solid solution. In solid solution, electrical conductivity can be enhanced by optimizing carrier concentration through bandgap engineering while thermal conductivity can be suppressed by enhancing phonon scattering by atomic disorder and mass difference. In this study, the TE properties of SnSe-SnTe solid solutions were investigated. Mechanical alloying and spark plasma sintering were used to fabricate SnSe-SnTe samples. XRD analyses were used to identify phases of the samples, and the microstructure of each sample was observed by FE-SEM. The bandgap of each sample was determined from UV absorption spectrum and compared with the DFT calculation results. The change of ZT will be discussed in terms of the carrier concentration and the band structure, and the effect of Te substitution on the TE transport properties will be discussed.

(EMA-P015-2020) Dielectric Properties of Barium Titanate Based CompositesS. Balciunas^{*1}; A. Karpavicius¹; M. Ivanov¹; J. Banys¹; S. Wada²

1. Vilnius University, Faculty of physics, Lithuania
2. University of Yamanashi, Material Science and Technology, Japan

In the last few decades there has been a growing interest in lead free piezoelectric materials. The main driving force is limitations due to environmental concern. $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ (PZT) is the most commercially viable piezoelectric material due to its high piezoelectric constant. Unfortunately, it is lead-containing, thus falls under the restriction of RoHS. In literature, most studies are focused on preparing high quality solid solution or composites at high temperatures which is not always desirable. In our presentation broadband dielectric properties of BaTiO_3 (BT) based composites with core-shell structure in temperature range of 100 to 500 kelvins will be presented. The composites were prepared in two steps. BT, BiFeO_3 (BF), $\text{BaTiO}_3\text{-Bi}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3$ (BT-BMT) and $\text{BaTiO}_3\text{-Bi}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3\text{-BiFeO}_3$ (BT-BMT-BF) nanoparticles were compressed with TiO_2 (ratio 1 : 1) in to low density pellets. Further, disk-shape pellets were submerged into barium hydroxide ($\text{Ba}(\text{OH})_2$) for solvothermal solidification. In the end we obtain BT around BT, BF, BT-BMT and BT-BMT-BF particles. In such systems cores are stressed by barium titanate shell creating similar conditions as in morphotropic phase boundary (MPB), thus increasing dielectric and piezoelectric constants. We have investigated dielectric properties in broad frequency range systems where core is a good dielectric, a relaxor, a ferroelectric and a non-ferroelectric material.

(EMA-P016-2020) Ferroic Domain Continuity over Grain Boundaries

S. Mantri^{*1}; J. Daniels¹

1. UNSW Sydney, Materials Science and Engineering, Australia

Ferroelectric domain continuity over grain boundaries in polycrystals has been observed since the 1950s, however, the exact geometric conditions in which this occurs has not been published. In this paper, we have studied the probability of ferroelectric and ferroelastic domain continuity over entire five-dimensional (three for the misorientation and two for the grain boundary plane normal) grain boundary space in ferroics of tetragonal and rhombohedral symmetry. This is further extended to 3 dimensional computed polycrystal, wherein the statistical analysis of the domain percolation length i.e., the number of grains that a domain can percolate is calculated. It is then compared with a textured polycrystal. It is shown that 28.64% of the 5-dimensional grain boundary space permits ferroelectric domain continuity within $1P_s$ charge and 1° angular tolerance. For a modeled polycrystal of random texture, domains can percolate through a maximum of 3 grains with a probability of 100 of a million observations under the above-specified tolerance. This is shown to increase considerably upon texturing of the ceramic.

(EMA-SP017-2020) Fabrication of Lead-Free (K,Na)NbO₃ Piezoelectric Thin Films by Sputtering with Improved Electromechanical Response

M. Waqar^{*1}; K. Yao²; S. J. Pennycook³; J. Wang³

1. National University of Singapore, NUS Graduate School for Integrative Sciences and Engineering, Singapore
2. A*STAR (Agency for Science, Technology and Research), Institute of Materials Research and Engineering (IMRE), Singapore
3. National University of Singapore, Department of Materials Science and Engineering, Singapore

Piezoelectric thin films have various applications in sensors, transducers and micro-electromechanical systems (MEMS). There have been recent breakthroughs in (K, Na)NbO₃ (KNN) based ceramic system which is among the most promising lead-free candidates for piezoelectric applications, however, such development and understanding have not been followed in KNN thin films. Deviation from compositional stoichiometry due to the high volatility of alkali species results in crystalline defects and secondary phase in these films. High-quality KNN epitaxial thin films with improved piezoelectric properties have been developed in this work using RF sputtering. The crystal structure and chemical composition of the obtained films are characterized using X-ray diffraction (XRD) and energy dispersive spectroscopy (EDS) respectively. Scanning Transmission Electron Microscopy (STEM) is employed to study the nature of crystalline defects on atomic scale. Laser scanning vibrometer (LSV) is used to determine the effective piezoelectric strain coefficient (d_{33}^*) of 77.4 pm/V. Dielectric constant and dielectric loss with the values of 526 and 0.05 respectively are achieved in these films measured using an impedance analyzer. The enhanced dielectric and piezoelectric properties are attributed to the improved crystalline quality of thin films due to the better control over stoichiometry.

(EMA-SP018-2020) Pulsed Laser Deposition of Lithium Cobalt Oxide Single Crystal Films

K. Glibe^{*1}; A. Sehrioglu²

1. Case Western Reserve University, Materials Science and Engineering, USA
2. Case Western Reserve University, USA

Layered oxides when dimensionally reduced can show unique properties such as superconductivity and changes in magnetism. When grown epitaxially, in addition to exhibiting structure-property relationships different from the bulk, the heterointerface can also provide unique properties. The layered oxide studied in this work

is LiCoO₂ (LCO) which is a common cathode material in Li-ion batteries. Therefore, both its electronic and ionic transport properties are of interest. LCO films were grown using pulsed laser deposition on top of an SrRuO₃ buffer layer and an SrTiO₃ substrate. By varying the oxygen pressure in the deposition chamber, temperature of the substrate, laser pulse rate, and fluence, the growth modes of the SrRuO₃ films were shown to change. In situ reflective high energy electron diffraction (RHEED) was used to verify the characteristics of film growth. The intensity distribution across each RHEED spot was analyzed over time for samples of different crystalline qualities. Additionally, Atomic Force Microscopy was used to examine the surface features of the films, and X-Ray Photoelectron Spectroscopy and Secondary Ion Mass Spectroscopy were used to determine the composition, especially the presence of Li in the films. The structures of the films were studied by X-Ray Diffraction based techniques. The epitaxial relationship between the films was analyzed.

(EMA-P019-2020) Sr-vacancy-controlled ferroelectricity in SrTiO₃ epitaxial thin films

K. Kang^{*1}; H. Seo²; O. Kwon²; K. Lee³; J. Bae⁴; M. Chu⁵; S. Chae³; Y. Kim²; W. Choi⁶

1. Los Alamos National Lab, USA
2. SungKyunKwan University, Republic of Korea
3. Seoul National University, Republic of Korea
4. Korea Basic Science Institute, Republic of Korea
5. National Taiwan University, Taiwan
6. SungKyunKwan University, Physics, Republic of Korea

SrTiO₃ is one of the most widely studied perovskite oxides owing to its incipient ferroelectric behavior. The incipient ferroelectric SrTiO₃ has exhibited the extraordinary high dielectric constant accompanying the significant temperature dependence. Employing various epitaxy techniques such as epitaxial strain, oxygen isotope exchange, and dimensionality, one can introduce the ferroelectric transition in SrTiO₃ thin film at finite temperature. Here, owing to the state-of-the-art pulsed laser epitaxy, we look into selective engineering of elemental vacancies for the systematic control of the ferroelectricity within epitaxial SrTiO₃ thin films. Therein, the control of Sr vacancy gives rise to the introduction and systematic change of the cubic-to-tetragonal transition, resulting in the inversion symmetry breaking necessary for the robust ferroelectricity at the room-temperature. Additionally, the tetragonality goes up with the increase in the Sr vacancies, eventually leading to the ferroelectricity enhancement. Our research summarizes the tetragonality-induced ferroelectricity in SrTiO₃ and provides functional growth control of the emergent phenomena.

(EMA-SP020-2020) Piezoresponse Predictions in Novel Ferroelectric Nanostructures

V. T. Reichelderfer^{*1}; L. Kuna¹

1. University of Connecticut, Materials Science and Engineering, USA

Here we present the results of a computational investigation in which the electroactive properties of sub-micron sized ferroelectric nanostructures are studied. Our computational approach involves finite element method (FEM) based simulations utilizing phenomenological Landau-Ginzburg-Devonshire theory, implemented in the open-source software package Ferret. We employ this approach to (a) benchmark our calculations for the piezoelectric properties of ferroelectric nanostructures against data found in literature and (b) propose novel nanostructures that could potentially have enhanced piezoelectric and electroactive properties. Our computational method predicts an enhancement of the piezoelectric d_{33} coefficient of one-dimensional PMN-PT nanostructures which is in excellent agreement with the results of experimental PFM measurements. Using these results as a benchmark, the piezoresponse of more complex structures, such as pyramids and patterned nanobelts, have also been investigated and will be presented.

(EMA-SP021-2020) Study of Perovskite and Spinel Complex Oxide Films and Nanocomposites Grown for Catalytic BehaviorR. Paudel^{*1}; R. B. Comes¹; M. Blanchet¹; A. Burton²; B. Farnum²

1. Auburn University, Physics, USA
2. Auburn University, Chemistry, USA

Complex metal oxides have attracted great deal of interest among researchers for their catalytic behavior. There is evidence that spinel and perovskite-type complex oxides exhibit highly efficient catalytic performance for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). The charging-discharging of hydrogen fuel cells are mediated by ORR and OER. Typical catalysts used in these reactions are usually the expensive metals like Pt, Ir. Complex metal oxides can provide a better low-cost alternative for those expensive metals. Our goal is to grow perovskite-spinel nanocomposite which serves as efficient bi-functional electrocatalyst for ORR and OER. We have successfully grown perovskites such as LaNiO_3 and LaCoO_3 and spinels such as CoMn_2O_4 , NiMn_2O_4 using molecular beam epitaxy. Grown films were examined for chemical composition and valency via in-vacuo x-ray photoelectron spectroscopy without being exposed to atmosphere. In addition, cyclic voltammetry and electrochemical impedance measurements were performed to understand the catalytic behavior of the oxide films. We will also show preliminary results on the synthesis of nanocomposites combining spinel and perovskite oxides.

(EMA-P023-2020) Effect of low energy ion irradiation on the properties of superconducting iron pnictide and magnesium boride thin filmsM. Nazir¹; Z. Xu³; N. Peng²; R. P. Webb²; D. Zheng^{*1}

1. Institute of Physics Chinese Academy of Sciences, China
2. University of Surrey, United Kingdom
3. Institute of Electrical Engineering Chinese Academy of Sciences, China

Ion irradiation is an effective method in producing defects so as to improve the pinning properties in superconductors. In this presentation, we show the results of ion irradiation on superconducting iron pnictide and magnesium boride thin films with relatively low energy (about a few hundreds keV). We irradiated high quality $\text{BaFe}_{1.84}\text{Co}_{0.16}\text{As}_2$ thin films, prepared by PLD, using 600 keV He^+ ions. Upon irradiation, the critical temperature T_C drops slightly while J_C is increased for samples with irradiation levels below $5 \times 10^{13} \text{ cm}^{-2}$. The analysis of the dependence of pinning force on magnetic field shows that the pinning behavior is not changed in the irradiated samples, suggesting more pinning centers of similar nature to those presented in the unirradiated samples are introduced by the irradiation process. The effects of 300 keV O^{+2} ion irradiation on the J_C in epitaxial MgB_2 thin films have also been studied. Again, we found that J_C is enhanced and its performance in magnetic fields is significantly improved. The scaling behavior reveals that the flux pinning mechanism evolves from grain-boundary-like pinning in the pristine and lightly irradiated films, to point-like pinning in moderately irradiated films, and again to grain-boundary-like pinning in heavily irradiated films.

(EMA-P024-2020) Length scale dependence of the structure of $(1-x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3-x\text{PbTiO}_3$ via pair distribution functionsA. Paterson^{*1}; A. Goetzee-Barral²; A. N. Johnson³; A. J. Bell⁴; M. Dolgos¹

1. University of Calgary, Chemistry, Canada
2. University of Leeds, United Kingdom
3. Oregon State University, USA
4. University of Leeds, Institute for Materials Research, United Kingdom

$\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ (NBT) is a relaxor ferroelectric material that has been heavily studied as an alternative to lead-based materials. In this work, the $(1-x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3-x\text{PbTiO}_3$ (NBT-PT) solid solution is examined as a model system to study the effect of lead on NBT, a disordered lead-free system. PT is a normal ferroelectric. Nano-scale domains have been reported in NBT-PT, but with increasing PT

content, macroscale domains arise. This work studies the differences between the local and average structure. NBT itself has been shown to have a hierarchical structure; differences in the structure appear depending on the length scale over which the structure is observed. For NBT-PT, X-ray and neutron diffraction measurements of the average structure reveal a rhombohedral R3c phase for $x = 0.08$, and a tetragonal P4mm phase for $x = 0.14$ and 0.18 . However, local structure analysis via pair distribution functions (PDFs) shows a length-scale dependent structure: these compositions show agreement with the monoclinic Cc phase at low-r length scales, but unit cell parameters approach average structure values observed by diffraction at increasing length-scales. The monoclinic phase only appears at short-ranges and is suppressed with increased PbTiO_3 content.

(EMA-P025-2020) Relaxor behavior and electrothermal properties of Sn and Nb modified $(\text{Ba,Ca})\text{TiO}_3$ Pb-free relaxor ferroelectricsS. Nayak^{*1}; S. Venkateshwarlu¹; F. Marlton²; F. Weyland³; N. Novak⁴; D. Maurya⁵; Y. Veerabhadraiah¹; O. Borkiewicz⁶; K. Beyer⁶; M. Jørgensen²; A. Pramanick¹

1. City University of Hong Kong, Department of Materials Science and Engineering, Hong Kong
2. Aarhus University, Interdisciplinary Nanoscience Center, Denmark
3. Institute of Materials Science, Germany
4. Jozef Stefan Institute, Slovenia
5. Virginia Tech, Department of Materials Science and Engineering, USA
6. Argonne National Laboratory, USA

Relaxor ferroelectrics are among the most successful electronic ceramics due to their highly attractive dielectric, piezoelectric, pyroelectric and electrocaloric properties. In this work, we synthesized a solid solution of Nb and Sn doped $(\text{Ba,Ca})\text{TiO}_3$ that exhibits relaxor-like properties with maximum permittivity near room temperature. The relaxor-like behavior of the ceramics is confirmed from dielectric spectroscopy, specific-heat capacity and piezo-force microscopy measurements. Two anomalies were observed from the dielectric permittivity spectrum: a peak ~ 300 K and a broad shoulder ~ 270 K. These two anomalies are correlated to temperature dependent changes in the average crystal structure and medium range (~ 1 nm) atomic correlations, respectively. The pyroelectric coefficient and electrocaloric properties for this material are presented. Interestingly, Nb and Sn doped $(\text{Ba,Ca})\text{TiO}_3$ ceramics exhibit a large pyroelectric coefficient of $(\partial P/\partial T) \sim 4000 \text{ -Cm}^{-2}\text{K}^{-1}$ near $T_s \sim 270$ K, followed by $(\partial P/\partial T) \sim 900 \text{ -Cm}^{-2}\text{K}^{-1}$ in the range of 275 - 325 K. It is therefore shown that length-scale specific structural changes can be induced in this material for pyroelectric energy harvesting. The study also demonstrates a new path for exploring relaxor properties in Pb-free compounds by incorporating dopants to facilitate co-operative multi-site atomic displacements.

(EMA-SP026-2020) Microstructural and Compositional Effects of Lithium Content on Perovskite $\text{La}_{1-x}\text{Li}_x\text{TaO}_3$ Ion ConductorsI. A. Brummel^{*1}; H. J. Brown-Shaklee²; J. Ihlefeld³

1. University of Virginia, Materials Science and Engineering, USA
2. Sandia National Laboratories, USA
3. University of Virginia, Department of Materials Science and Engineering, USA

We present a methodology for the preparation of perovskite $\text{La}_{1-x}\text{Li}_x\text{TaO}_3$ (LLTO), $x=0.33$, lithium ion conductors based on combustion synthesis. Bulk ceramic specimens were prepared under different lithium overpressure and lithium excess conditions governed by combinations of burial powder, enclosed crucibles, and batching. Specimens were sintered at 1500°C with nominal lithium excess ranging from 10-30 at%, to account for sintering losses. A lithium-ion conductivity maximum was observed as a function of the post-sintering lithium content with a maximum value of $6 \times 10^{-6} \text{ S/cm}$. Maximal values in both the inter- and intra-granular

ion conductivity occurred under the same conditions. To explore a possible Schottky barrier effect at grain boundaries, impedance spectroscopy was performed with differing DC bias conditions. The lithium-ion conductivity was found to be independent of applied DC bias, implying grain boundary conductivity effects are not governed by Schottky barriers. All specimens were observed to exhibit tetragonal symmetry. The effect of grain size in the ceramics were found to influence the lithium-ion conductivity, with increased grain size leading to increased overall ionic conductivity. The results will be presented in the context of other ion conducting systems where microstructure affects performance.

(EMA-SP027-2020) Nano-Porous Niobium Oxide Formed Via Electrochemical Anodization as a Negative Electrode for Sodium-ion Batteries

P. Barnes¹; K. E. Dixon^{*1}; B. Bernal¹; H. Xiong¹

1. Boise State University, Materials Science and Engineering, USA

Increasing demand for renewable energy sources is driving the need for electrochemical energy storage systems. The Li-ion battery is the most prominent energy storage technology today capable of meeting this demand. However, Li is relatively rare and has various obstacles to its production. Therefore, a more abundant and less expensive alternative is appealing. Sodium is an attractive alternative to lithium as it offers a more sustainable outlook. However, its larger ionic radius and mass have reduced its implementation to electrochemical energy storage. Differences exist between Na and Li ion battery chemistry. For example, the larger Na ion slows diffusion rates, which limit electrochemical performance, and causes stress/strain in the host material. Therefore, finding intercalation hosts, capable of facilitating ionic and electronic transport becomes paramount. Niobium oxide is one such option. It possesses a variety of crystalline structures, which could be capable of a topotactic reaction. Additionally, nano-porous thin films can be formed, providing shorter pathways for electrolyte penetration and charge transport. In this work, nano-porous niobium oxide was formed via a facile anodization process, where conditions were tuned to produce a variety of pore sizes. The nano-porous niobium oxide was then evaluated as a negative electrode in a sodium ion battery.

(EMA-SP028-2020) Processing and characterization of LTO-Ni-LLTO composite anodes

W. Huddleston^{*1}; F. Dynys²; A. Sehrioglu³

1. Case Western Reserve University, Department of Materials Science and Engineering, USA
2. NASA Glenn Research Center, USA
3. Case Western Reserve University, USA

In this study, multifunctional composites of strain-free $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO), nickel metal current collector, and lithium conducting electrolyte $\text{Li}_{0.3}\text{La}_{0.56}\text{TiO}_3$ (LLTO) was investigated to enable next generation aerospace concepts. This anode-supported structural battery must provide high electronic and ionic conductivity and maintain structural integrity for simultaneous electrochemical and mechanical performance to achieve systems-level weight savings. Processing-property-performance relationships were explored for LTO-Ni-LLTO three phase composites to meet these requirements. Processing routes were identified that reached the high sintering temperatures necessary for densification, enabled the recovery of the low temperature cubic spinel phase, and ensured the internal reduction of current collector particles after densification. Dense electrodes with bulk electrical conductivity >1 S/cm were achieved by sintering in air and reducing atmospheres with only 13 vol.% nickel. Analysis of electrochemical capacity, cycling, and rate capability were combined with measurements of mechanical fracture strength for evaluation of multifunctional performance as a function of composite composition and sintering conditions.

(EMA-SP035-2020) Stable high permittivity and low dielectric loss of Ce-doped SrTiO_3 ceramics

J. Qi^{*1}; C. Randall¹

1. Pennsylvania State University, Materials Research Institute, USA

High permittivity and low dielectric loss can be achieved in Ce-doped SrTiO_3 ceramic samples simultaneously ($\epsilon_r=7070$, $\tan\delta=0.007$ at RT and 1kHz). Here, we found that: A portion of Ti^{3+} was detected in the high temperature air-sintered sample, and the Ti^{3+} ions lead to the Ti-O octahedral off-center, which make a certain contribution to improve the intrinsic dielectric constant; Due to the defect complex is energetically favored over the isolated defects, defect-complex (i.e. $\text{Ti}^{3+}-\text{V}_o-\text{Ti}^{3+}$; $\text{V}_{\text{Sr}}-\text{V}_o$) could be suppress the dielectric loss relaxation caused by the motion and ionization of V_o . Follow this line of thought, a further enhanced dielectric properties can be achieved in reducing atmosphere sintering sample ($\epsilon_r=12650$, $\tan\delta=0.006$). Further investigation of this unique dielectric response will be considered.

(EMA-SP029-2020) Thermal properties of ZrB_2 and $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Ta}_{0.2}\text{Nb}_{0.2})\text{B}_2$

M. Hoque^{*2}; J. L. Braun²; J. Gild³; D. Olson²; K. Aryana²; J. Tomko⁴; Y. R. Koh²; R. Galib²; J. Gaskins²; W. Fahrenholtz²; J. Luo⁶; P. E. Hopkins¹

1. University of Virginia, Department of Mechanical and Aerospace Engineering, Department of Materials Science and Engineering, Department of Physics, USA
2. University of Virginia, Mechanical and Aerospace Engineering, USA
3. University of California, San Diego, Materials Science and Engineering Program, USA
4. University of Virginia, Department of Materials Science and Engineering, USA
5. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA
6. University of California, San Diego, USA

Thermal conductivity and heat capacity of Zirconium diboride (ZrB_2) and a high entropy boride $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Ta}_{0.2}\text{Nb}_{0.2})\text{B}_2$ from room temperature to 300 °C are reported. Thermal properties of the two refractory borides are characterized by four different techniques, namely time domain thermoreflectance (TDTR), steady-state thermoreflectance (SSTR), TDTR mapping and hot disk. Thermal conductivity measured by recently developed optical pump-probe technique SSTR are in excellent agreement with hot-disk and literature values. The room temperature thermal conductivity of ZrB_2 is $137.3 \pm 9.7 \text{ Wm}^{-1}\text{K}^{-1}$, and a six fold decrease is achieved in $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Ta}_{0.2}\text{Nb}_{0.2})\text{B}_2$ to $23.7 \pm 1.5 \text{ Wm}^{-1}\text{K}^{-1}$. The volumetric heat capacity of the bulk borides is measured by two approaches: frequency dependent TDTR and a combination of SSTR and TDTR. The high entropy boride possesses a volumetric heat capacity of $2.9 \pm 0.4 \text{ MJm}^{-3}\text{K}^{-1}$. TDTR mapping revealed the possible influence of grain orientation and local defect phases on the thermal properties of borides over a large area. The lower thermal conductivity and higher heat capacity of the high entropy boride make it unique for potential application as a structural ceramic.

(EMA-SP030-2020) Study of ultrafast carrier dynamics in GaAs by mid-IR pump-probe spectroscopy

R. Galib^{*1}; J. Tomko²; D. Olson¹; J. Gaskins¹; P. E. Hopkins¹

1. University of Virginia, Mechanical and Aerospace Engineering, USA
2. University of Virginia, Materials Science and Engineering, USA

Ultrafast laser spectroscopy is a versatile technique that is commonly used to both understand and manipulate electronic scattering mechanisms in semiconductors. The processes that drive electron scattering have major implications from both technological and scientific perspectives. For example, a key challenge in optoelectronic devices, such as light emitting and laser diodes, is enhancement of the active region's internal quantum efficiency, which is reduced by various nonradiative recombination processes.

While previous works have been able to elucidate generalized scattering rates through visible probing of excited materials, the use of optical wavelengths is only capable of investigating interband scattering times due to the high energy photons. In this work, we develop a sub-picosecond optical pump, mid-infrared probe system to directly interrogate intraband/intervalley electron scattering mechanisms of GaAs. Our measurements provide direct evidence that excited electrons decay at greatly different rates based on their energy relative to the conduction band minimum. These findings provide additional insight into the energy-dependent nature and rate of phonon emission during electronic relaxation. Additionally, we find that mid-gap defect states, which are intrinsic to undoped GaAs, have greatly reduced relaxation times relative to the intrinsic scattering processes within the conduction band.

(EMA-SP031-2020) Two-dimensional CuI on Cu(111): A first-principles investigation

G. Lee^{*1}; T. Lee¹; A. Soon¹

1. Yonsei University, Department of Materials Science & Engineering and Center for Artificial Synthesis Materials Discovery, Republic of Korea

Of late, copper iodide (CuI), a p-type transparent semiconductor at room temperature, has been proposed as a choice material for various potential applications – from a hole conductor to a bipolar diode, forming a two-dimensional heterojunction with various n-type materials. However, the controlling the atomic structure of ultrathin (or interfacial) CuI layers for these targeted applications is challenging due to the existence of various polymorphic expressions. The structures of ultrathin layers are determined by the orientation of metal substrates (e.g. Cu(100) and Cu(111)) and the surface coverage of precursors (e.g. I₂ (g) or KI (aq)) used. In this work, we have performed *ab initio* density-functional theory calculations to examine the initial/early stages of CuI ultrathin film formation on Cu(111) within the framework of *ab initio* atomistic thermodynamics, and report detailed surface atomic structures with their associated surface thermodynamics and simulated scanning tunneling microscopy images. Here, we find that due to the unique atomic arrangements in the ultrathin CuI film, both charge transfer and polarization effects to the surface work function are pronounced and contribute to its surface electronic structure as captured in the electronic charge density differences at the interface.

(EMA-P032-2020) Development of the algorithm for automatic, reliable, and high-throughput structural refinement method using the Rietveld analysis

A. Aimi^{*1}; K. Fujimoto¹

1. Tokyo University of Science, Pure and Applied Chemistry, Japan

The collection of crystallographic information for various compounds is helpful for material design. Rietveld analysis is mainly used for obtaining crystallographic parameters from powder X-ray/neutron diffraction data. However, there are various difficulties to collect reliable crystallographic information. Obtained results are influenced by the refinement procedure, and thus analysts are required high time, labor and expertise in crystallography. To overcome these problems, a novel algorithm to automate the Rietveld analysis was developed in this study. The feature of algorithm is the repeating of generation a set of initial values and one-shot refinement, as opposed to manual analysis, which use a single set of initial values and refine step by step. The program was written in C++ language. The RIETAN-FP software was used as the engine for nonlinear least-squares pattern fitting. The XRD data of CaMnTi₂O₆ were analyzed automatically. When random generation of a set of initial values and one-shot analysis were repeated until converged results obtained 1000 times, reasonable fitting results were obtained 33 times. The required time for automatic analysis was about 1/5 with respect to that for manual analysis. This method counts for high-throughput material research by reducing the labor and time for Rietveld analysis.

(EMA-SP033-2020) Design of novel molecular ferroelectrics using first-principles based and machine learning approaches

A. Ghosh^{*1}; L. Louis¹; K. Pitike¹; S. Poddar²; S. Ducharme²; A. Asandei¹; N. Lubbers³; S. Nakhmanson¹

1. University of Connecticut, Materials Science and Engineering, USA
2. University of Nebraska, Lincoln, USA
3. Los Alamos National Lab, USA

Recent advances in the synthesis of polar molecular materials have produced viable alternatives to ferroelectric ceramics opening up exciting new avenues for the incorporation of such compounds into modern electronic devices. Polyvinylidene fluoride (PVDF) is a well-known multifunctional polymer with outstanding polar, pyroelectric and ferroelectric properties. This presentation will illustrate how a density-functional theory approach, combined with the Modern Theory of Polarization formalism utilizing maximally-localized Wannier functions is used to investigate the electronic origins of ferroelectricity in two distinct classes of polar molecular materials: PVDF-based mixed polymer crystals incorporating 2,3,3,3-tetrafluoropropene (TFP) and molecular cocrystals containing combinations of diisopropylammonium (DIPA) units with different halide counter ions. Moreover, the same DFT-guided principles can be used as a backbone for data mining and machine learning methods to explore a broad chemical space of molecular materials, identify specific traits pointing toward ferroelectric behavior and incorporating experimental observations in a high-throughput manner.

(EMA-SP034-2020) Heterojunction properties of MPS/PANI doped with erbium

R. P. Toledo^{*1}; A. F. Oliveira¹; D. R. Huanca¹

1. Federal University of Itajubá, Institute of Physics & Chemistry, Brazil

Silicon is the predominant material in semiconductor devices field. Their physical and chemical properties can be tuned by including pores inside the bulk. Despite its indirect band gap, the porous silicon (PS) has been employed in the fabrication of optoelectronic devices with wavelength light ranging in the visible region because its luminescence properties, which rises due to the confinement effect in crystallites with effective diameter shorter than 5 nm. However, for some applications emission light with wavelength in the infrared region is desirable, like in the information transfer field which happens at 1.53 μm. Unfortunately, light emission with this wavelength was not reported until now. The suggested strategy to overcome this difficulty is to employ erbium ions as doping element of PS. In this sense, some research groups have investigated the erbium doped PS (PS:Er) as function of the Er concentration and fabrication parameters. This aim was achieved by anodizing p-type Si in HF:DMF, and then PANI was deposited by cyclic voltammetry (CV). After, this method was also used to include Er ions into PANI. The presence of PANI was confirmed by FTIR analysis reveals that PANI was deposited in its most conductive state. The measurements of current and impedance were made at different points. Thus, the results showed that the sample has properties for application in photonic devices.

(EMA-SP036-2020) Ferroelectric Domain Switching in BFO/CFO Vertically Aligned Nanocomposites as a Function of Epitaxial Interface Proximity and Magnetic Poling

L. Ortiz^{*1}; M. Martin¹; J. Song¹; A. Chen²; B. Huey¹

1. University of Connecticut, Materials Science and Engineering, USA
2. Los Alamos National Lab, USA

Vertically epitaxial nanocomposites of BiFeO₃ and CoFeO₃ are promising as multiferroics due to the extraordinarily high area density of strained BFO/CFO interfaces. This work investigates correlations between ferroelectric switching in the BFO and distance from the phase boundary based on piezo-force microscopy. This reveals no preference for nucleation near interfaces for low voltages, and an increasing correlation as switching fields increase. Magnetic domains in the CFO phase are also imaged via magnetic force microscopy, respectively. Work to resolve ferroelectric and magnetic domains before and after magnetic poling is ongoing.

Thursday, January 23, 2020

Plenary Session II

Room: Orange A

Session Chair: Wolfgang Rheinheimer, Purdue University

8:40 AM

(EMA-PLEN-002-2020) Defect Disorder and Dynamics in Functional Oxides

E. C. Dickey*¹

1. North Carolina State University, Materials Science and Engineering, USA

Lattice defects play an important role in the dielectric and conductivity properties of ceramic materials, and thus great effort is expended on controlling point defect equilibria via doping, oxygen activity and temperature control during processing. In device applications, because lattice defects are typically charged, applied electric fields provide a strong driving force for defect migration, and their spatio-temporal redistribution depends on the electric potential distribution and the interfacial exchange kinetics. Ultimately this process leads to spatially varying conductivity profiles and often a concomitant macroscopic increase in leakage current in many dielectric materials. While this leakage current enhancement is detrimental in devices such as capacitors, the phenomenon can be utilized to form novel functional behaviors such as resistive switching in metal-oxides. Furthermore, the use of electric fields in processing ceramic materials, e.g. flash sintering, can lead to analogous electromigration processes resulting in long-range chemical and microstructural gradients. This talk will review our current understanding and implications of point defect electromigration in important electroceramic materials.

S1: Characterization of Structure-Property Relationships in Functional Ceramics

Probing Defects and Disorder in Functional Ceramics

Room: Citrus B

Session Chair: James LeBeau

10:00 AM

(EMA-S1-013-2020) Structural insights into the depolarization processes in sodium bismuth titanate based piezoelectrics (Invited)

G. Adhikary¹; A. Mishra¹; D. K. Khatua¹; R. Ranjan*¹

1. Indian Institute of Science, Materials Engineering, India

While the surge in lead-free piezoelectric research in the last decade and a half have led to the discovery of new lead-free piezoelectric compositions with large electromechanical properties, it also threw new challenges regarding understanding the structure-property correlations in these systems. In contrast to the BaTiO₃ and (K,Na)NbO₃ based lead-free piezoelectrics, the complexity associated with the inherent structural disorder on the local scale of Na_{0.5}Bi_{0.5}TiO₃ (NBT) pose serious challenges to the understanding of structure-property relationships in NBT based piezoceramics. In this presentation three important issues associated with NBT based piezoceramics will be addressed: (i) the anomalous drop in the depolarization temperature at the morphotropic phase boundary, (ii) the subtle nature of the structural transformation associated with thermal depolarization at the MPB, and (iii) structural insight into the phenomenon of thermal depolarization delay in some modified NBT-piezoceramics. We show that the anomalous dip in the depolarization temperature is intimately associated with the

system's strong propensity for stabilizing non-ferroelectric distortion on approaching the MPB. We also show a correspondence between grain size, ferroelectric lattice distortion, and depolarization temperature in these systems.

10:30 AM

(EMA-S1-014-2020) Study of local structure of Dion-Jacobson phases with hybrid improper ferroelectricity

J. Kong¹; S. Nayak¹; A. Pramanick*¹

1. City University of Hong Kong, Department of Materials Science and Engineering, Hong Kong

The recent discovery of hybrid improper ferroelectricity (HIF) in layered perovskites has opened up new avenues for development of polar materials with expanded functionalities. The spontaneous polarization in HIF arises through a trilinear coupling between two or more non-polar lattice distortion modes involving antiferrodistortive tilting of oxygen octahedra and a polar lattice mode. Coexistence of structural instabilities arising from antiferrodistortive octahedral tilting and polar modes are common in many perovskites and previous studies have indicated that these instabilities can be either competitive or co-operative. The interaction between antiferrodistortive octahedral tilts and polar displacements can also give rise to local structural deviations, which become important for determining the macroscopic properties. In contrast, the nature of interaction between antiferrodistortive octahedral tilts and polar mode displacements in layered perovskites with HIF are currently not well understood. In this talk, I will present results from our recent study of temperature-dependent local structural evolution in Dion-Jacobson layered perovskites, CsBiNb₃O₇ and Cs(Bi,La)Nb₂O₇, using X-ray pair distribution function (PDF). It will be shown that interactions between the polar and the octahedral tilting/rotational modes in these Dion-Jacobson phases are competitive at lower temperatures.

10:45 AM

(EMA-S1-015-2020) Unusual Trends in the Enhanced Ce³⁺ Surface Concentration in Ceria-Zirconia Catalyst Materials (Invited)

W. Yuan¹; Q. Ma²; I. Takeuchi³; M. Bedzyk¹; S. M. Haile*¹

1. Northwestern University, Materials Science and Engineering, USA
2. Northwestern University, Synchrotron Research Center, USA
3. University of Maryland, USA

Despite the immense importance of ceria-zirconia solid solutions in catalysis, the extent of reduction at the surfaces of these materials, and hence the concentration of reactive Ce³⁺ species, is unknown. Using angle-resolved X-ray Absorption Near Edge Spectroscopy (XANES), we quantify under technologically relevant conditions the Ce³⁺ concentration in the surface (2-3 nm) and bulk regions of ceria-zirconia films grown on YSZ(001). In all circumstances, we observe substantial Ce³⁺ enrichment at the surface. For example, in CeO_{2-x} at 1100 °C and $\approx 3 \times 10^{-6}$ atm oxygen partial pressure the surface Ce³⁺ concentration is a remarkable 62%. This stands in stark contrast to the results of thermogravimetric measurements which indicate the bulk concentration of such species under these conditions is negligible. The trends with Zr concentration are even more surprising. It is well known that the bulk Ce³⁺ concentration and hence oxygen vacancy concentration increases upon introduction of Zr. Here, we find that, although surface enhancement of the Ce³⁺ concentration persists, the degree to which the surface differs from the bulk decreases monotonically with Zr concentration. Thus, the fraction of cations in the 3+ state at the surface of the materials drops steeply as Zr is introduced. The relevance to surface reaction rates is discussed.

11:15 AM

(EMA-S1-016-2020) X-ray Absorption Spectroscopy Studies of the Oxide-ion Conduction Mechanism in Sodium bismuth titanate ($\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$) based perovskitesM. Lucero^{*1}; C. M. Culbertson²; R. McQuade²; A. Paterson³; M. Dolgos²; D. Cann⁴; Z. Feng¹

1. Oregon State University, School of Chemical, Biological and Environmental Engineering, USA
2. Oregon State University, Department of Chemistry, USA
3. University of Calgary, Chemistry, Canada
4. Oregon State Univ, School of Mechanical, Industrial, and Manufacturing Engineering, USA

It has been observed that sodium-bismuth titanate based perovskites $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT) exhibit oxide ion conduction with comparable conductivity with the state-of-the-art ion conductors (e.g. $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95}$). These materials are promising candidates as high-performance oxide conductors for solid oxide fuel cells with reduced cost. However, the mechanism of high conductivity is unclear. It is suspected that the local structure disordering could be the source of the superior performance. Therefore, we use both hard (hXAS) and soft (sXAS) X-ray absorption spectroscopy to probe the local structure as a function of composition and temperature. The Bi L-edge, Ti L-edge, and O K-edge have been measured for stoichiometric, non-stoichiometric, and Mg & Nb doped NBT. We found that at room temperature there is no significant change in the spectral line shape for the three edges indicating that the electronic and local structure does not change when the NBT is bismuth deficient or doped. However, these measurements were performed at room temperature whereas the phenomenon of oxide conductivity is observed at higher temperatures. A multi-edge (e.g. Bi L, Ti L, O K and Nb K edges) study as the function of temperature (30-700 °C) is performed using both hXAS and sXAS to probe the local structural changes at temperature.

S2: Advanced Electronic Materials: Processing Structures, Properties, and Applications

Lead-free and Relaxor Ferroelectrics

Room: Orange B

Session Chair: Ke Wang, Tsinghua University

10:00 AM

(EMA-S2-017-2020) Effect of AC electric field poling on relaxor-PT crystals (Invited)F. Li^{*1}

1. Xi'an Jiaotong University, China

Electric poling that aligns the internal polar regions (domains) within the ferroelectric is the key step to turning ferroelectrics into an electromechanically active materials with numerous applications. Relaxor- PbTiO_3 crystals, being an important class of ferroelectrics, possess ultrahigh piezoelectricity when compared with state-of-the-art $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$ ceramics. Recently, an even higher piezoelectricity is observed in alternating current electric-field-poled (AC-poled) relaxor- PbTiO_3 crystals when compared to traditional DC-poled counterparts. In this presentation, I will introduce recent researches on AC-poled relaxor-PT crystals, including the scaling effect and the origin of enhanced piezoelectricity of AC-poled crystals. Compared with the traditional poling method, the piezoelectric coefficient (d_{33}) was found to be increased by 20%-35% via AC-poling. Minimal scaling effect was observed for the samples with thickness above 200 μm . While, for 100- μm samples, the dielectric permittivity was only enhanced by 6%, and a clear degradation of properties was observed when the cycle of alternating current electric

field is beyond three. These features are thought to be associated with the impacts of surface damages for thin samples. With a combination of phase field simulations and experimental characterizations, I will summarize the impacts of AC-poling on domain structures and properties of relaxor- PbTiO_3 crystals.

10:30 AM

(EMA-S2-018-2020) Ceramics fractal nature influence on BaTiO_3 - nano scale and dielectric properties towards coated morphology processingV. Mitic^{*1}; G. Lazovic²; C. Lu³; V. Paunovic⁴; I. Radovic⁵; S. Veljkovic⁴; B. Vlahovic⁶

1. Serbian Academy of Sciences /Faculty of Electronic Engineering University Nis, Institute of Technical Sciences, Serbia
2. University of Belgrade, Faculty of Mechanical Engineering, Serbia
3. Industrial Technology Research Institute, Taiwan
4. University of Nis, Faculty of Electronic Engineering, Serbia
5. University of Belgrade, Vinca Institute of Nuclear, Serbia
6. North Carolina Central University, USA

Perovskite ceramics are widely recognized and investigated as materials with great potential for the use in electronic industry. Because of their electronic properties, nano- BaTiO_3 perovskite has been the focus of our presented research. Nanopowder of BaTiO_3 has been coated with metal organic yttrium salt (MOD-Y) and Y_2O_3 , with sintering in the temperature range from 1200 to 1350C. This study presents novel approach for the investigation of electronic properties on the interface between BaTiO_3 grains. Transmission electron microscopy demonstrated around grains new phase forming. DC capacitance measurements have revealed significantly higher Dk value for $\text{BaTiO}_3/\text{MOD-Y}$ compared to $\text{BaTiO}_3/\text{Y}_2\text{O}_3$. Grain boundary control mobility in DC Bias operation voltage and nano scale grain boundary control were related to temperature, while fractal nature characterization gave insight in the relations between grains, pore surface and particles' Brownian motions. All of these findings enlight new perspective to a control of the processing parameters, morphology and desired properties.

10:45 AM

(EMA-S2-019-2020) Inhomogeneous Poling-induced Phase Transitions in Potassium Sodium Niobate-based Piezoelectric ActuatorsS. Funni^{*1}; J. Zhao¹; E. C. Dickey¹; J. L. Jones¹

1. North Carolina State University, Dept. of Materials Science & Engineering, USA

Potassium sodium niobate (KNN) has been widely investigated for use as a lead-free piezoelectric in devices such as multilayer ceramic actuators (MLCAs). It is well known that voltages applied to an MLCA induce large electric field and stress concentrations near the electrode edges. A KNN sample with a full bottom and partial top electrode is used to approximate the geometry of an MLCA. In situ high-energy X-ray diffraction with an ultra-small beam size was performed at the Advanced Photon Source. The beam was scanned over the region near the electrode edge before, during and after application of a coercive electric field. Orthorhombic and tetragonal phase fractions at each stage of the experiment are extracted from this data. Coupled-physics finite element modeling (FEM) is used to simulate the mechanical and electric field states in the region near the electrode edge. The electrode geometry produces a poling field of non-uniform alignment, therefore accurate modeling requires the use of variably oriented material properties. Implementing this material model, FEM results are directly correlated with the experimental data to determine the driving forces for poling-induced phase change in KNN. This material is based upon work supported by the National Science Foundation, as part of the Center for Dielectrics and Piezoelectrics under Grant Nos. IIP-1841453 and IIP-1841466.

11:00 AM

(EMA-S2-020-2020) Dynamics of an interferroelectric phase transition in (011) PIN-PMN-PT crystals (Invited)

M. L. Staruch^{*1}; E. A. Patterson¹; P. Finkel¹; D. Damjanovic²; M. Cain³

1. US Naval Research Laboratory, USA
2. Swiss Federal Institute of Technology in Lausanne - EPFL, Ceramics Laboratory, Switzerland
3. Electrosiences Ltd., United Kingdom

Enhancement of piezoelectric properties near a morphotropic phase boundary is well known, and recent efforts have also focused on how to switch between these two phases using external stimuli. In particular, in (011) cut and poled $\text{Pb}(\text{In},\text{Nb})\text{O}_3$ - $\text{Pb}(\text{Mg},\text{Nb})\text{O}_3$ - PbTiO_3 (PIN-PMN-PT) single crystals near an MBP, a ferroelectric-ferroelectric rhombohedral to orthorhombic transition can be realized under stress, electric field, and/or temperature. This phase transition is associated with a large jump in polarization and strain. To evaluate the transduction properties of this non-linear phenomenon, both quasi-static and dynamic measurements of the piezoelectric coefficient d_{32} (or d_{32}^*) were made using several techniques. Although a general decrease with increasing frequency was observed, the values in the phase transitional regime were always $\sim 2x$ higher than in the linear rhombohedral or orthorhombic phases. Synchrotron x-ray diffraction (XRD) experiments were performed at a grazing incidence to look for potential skin effects under electric field and temperature. A significant difference in the peak shift, and therefore the effective piezoelectric coefficient, was observed in the first few nanometers of the film. Experimentation is also currently underway on a fixture to apply a dynamic stress in-situ to study the frequency dependence with XRD, and preliminary results will be presented.

Synthesis of Electronic Materials and the Role of Defects

Room: Orange B

Session Chair: Margo Staruch, US Naval Research Laboratory

2:00 PM

(EMA-S2-021-2020) Chemical Heterogeneity in (K, Na)NbO₃-based Piezoceramics: Good or Evil? (Invited)

K. Wang^{*1}; H. Thong¹; M. Zhang¹; J. Li¹

1. Tsinghua University, School of Materials Science and Engineering, China

Piezoelectric materials can be utilized in a variety of electronic devices, such as sensors, actuators, and transducers. However, the dominant materials used in these devices are lead zirconate titanate (PZT)-based, which are hazardous to human and environment. Therefore, the development of lead-free substitutions is economically and socially beneficial. Potassium sodium niobate (KNN)-based piezoelectric materials are the most outstanding and promising lead-free candidates. KNN-based piezoelectric materials have been being transferred from research into application in the past few years. However, poor reproducibility of KNN-based materials is a difficult problem to both industrial manufacturing and scientific research. In the present study, we discovered irregular grain growth, accompanied by chemical heterogeneity in the calcined KNN piezoceramic powder. The heterogeneous calcined powder was then subjected to the conventional sintering. Ferroelectric phase coexistence was observed in the sintered ceramic and was proposed to be dependent to the kinetic of calcination reaction. We conclude that the crystal structure of Nb_2O_5 will determine the structure and properties of KNN-based materials, and might account for the poor reproducibility.

2:30 PM

(EMA-S2-022-2020) Exploration and Synthesis of Novel PZT - based Ternary: BiInO₃ - Pb(Zr,Ti)O₃

J. Nikkel^{*1}; R. McQuade³; M. Dolgos²; D. Cann³

1. Oregon State University, Chemistry, USA
2. University of Calgary, Chemistry, Canada
3. Oregon State Univ, School of Mechanical, Industrial, and Manufacturing Engineering, USA

This study focused on the exploration and investigation of lead zirconate titanate (PZT) based ternary systems. As the ability to modify PZT systems to enhance desired properties, without significant impact to already established processing procedures, would be a direct boon to current technology and devices, elucidating novel ternary systems could be of great interest. Here the solid solution of BiInO_3 - PbZrO_3 - PbTiO_3 (x BI - (1/x) PZT) was explored focusing on fixed Zr/Ti ratios of 52/48 and 50/50. Through calcination studies, stable solid solutions were found up to 15% of BI for PZT 52/48, and up to 10% in PZT 50/50. Characterization was done on samples for $0\% \leq x \leq 10\%$ BI in PZT 52/48. These samples tended toward rhombohedral phase with increasing %BI. The Curie temperature of these samples decreased with increasing %BI from $\sim 390^\circ\text{C}$ in pure PZT 52/48 to 322°C in 10% BI. Ferroelectric and piezoelectric studies of the 2.5% BI sample showed a coercive field of 14.4 kV/cm, a $P_{\text{max}} = 38 \text{ mC/cm}^2$, $P_r = 29 \text{ mC/cm}^2$, and a $d_{33}^* = 248 \text{ pC/N}$ under a max applied field of 70 kV/cm at 1 Hz.

2:45 PM

(EMA-S2-023-2020) One pot synthesis of dielectric BaTiO₃ based nanocubes with heteroepitaxial interfaces by hydrothermal method

K. Mimura^{*1}; Z. Liu¹; H. Itasaka¹; K. Kato¹

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

We have developed barium titanate nanocubes (BT NCs) with high crystallinity and high dielectric properties in recent years. 3D assembly of BT NCs which was fabricated by capillary force assisted self-assembly process and post annealing achieved a high dielectric constant above 4000 with low loss values below 7 %. Numerical calculation and Raman spectroscopy revealed that the interface strains may be one possibility of high dielectric properties of BT NC assembly. Therefore, control of interfaces is one of the most important and effective to enhance the dielectric properties of nanomaterials. In this study, we focused on the fabrication of heteroepitaxial interfaces within the nanocube. Hetero-epitaxial interfaces are necessary to effectively express the special properties of nanomaterials such as high dielectric properties, piezoresponse, and so on. We directly synthesized perovskite-based nanocubes which include hetero-epitaxial interfaces inner part by one-pot hydrothermal method. The size of nanocubes was about 50-80 nm observed by SEM. STEM observations showed that BT-based core nanocrystal with tetragonal symmetry and cubic shaped another perovskite-based shell with orthorhombic symmetry were in hetero-epitaxy relation. This unique structure nanomaterial will be promising to utilize for next generation dielectric devices.

3:00 PM

(EMA-S2-024-2020) Properties of ZnO/Reduced Graphene oxide Quasi Core-Shell NanoparticlesA. Nemati^{*1}; S. P. Haghshenas¹; A. Simchi¹; C. Kim²

1. Sharif University of Technology, Department of Materials Science & Engineering, Islamic Republic of Iran
2. University of Texas at Arlington, Department of Materials Science & Engineering, USA

In this paper, zinc oxide, reduced graphene oxide and zinc oxide/reduced graphene oxide quasi core-shell nanoparticles were prepared. Zinc oxide was considered as a core and few layer of reduced graphene oxide as a shell on top of that, abbreviated as ZnO/RGO). After synthesizing of ZnO/RGO samples, the photocatalytic behavior of ZnO/RGO Quasi Core-Shell Nanoparticles as well as pure ZnO nanoparticles was tested and compared. Raman spectroscopy results confirmed ZnO formation at various temperatures but a little shift was observed for ZnO/RGO quasi core-shells nanoparticles after conjugating. Oxygen was the main reason for the connection between the core and the shell. Our results indicated that the rate of MB degradation (as a measure of photocatalytic behavior of the system) for ZnO/RGO quasi core-shell structures was less than pure zinc oxide. Our results indicated that how either band structure modification and defect chemistry or microstructural features can affect the photocatalytic behavior in a specific quasi core shell structure.

3:45 PM

(EMA-S2-025-2020) Detecting chemical and structural inhomogeneity in ferroelectric, relaxor and dielectric materials via impedance spectroscopy (Invited)T. Frömling^{*1}; Y. Liu¹; S. Steiner¹; A. Hoang¹; M. Gehringer¹; L. Kodumudi Venkatamaran¹; B. Xu¹

1. Technische Universität Darmstadt, Materials Science, Germany

In research of ferroelectric, relaxor and dielectric ceramics synthesizing solid solutions and using dopants are usually strategies to optimize functional properties. It is of high importance to know whether the samples are actually phase pure and whether the defect chemical properties are homogeneous. Otherwise it is impossible to attribute variations in functional properties to the changes of composition. XRD, SEM and EDX are the usual way to study the presence of secondary phases but are often not sensitive enough. Information on defect inhomogeneity, e.g. induced by rapid cooling or dopant segregation to the grain boundary, is usually not obtained. Hence, more complex investigations methods are usually required. In this work, methods based on simple frequency dependent electrical investigations will be revisited and extended to obtain qualitative and possibly quantitative information on variations in composition and defect chemistry. Furthermore, the impact of composite formation on the electrical response will be discussed.

4:15 PM

(EMA-S2-026-2020) Tunable Giant Electromechanical Properties in Defective Co-doped Ceria SystemsA. Kabir^{*1}; V. Esposito²

1. Technical University of Denmark, DTU Energy, Denmark
2. Technical University of Denmark, Denmark

Recent studies demonstrate that highly defective cerium oxide, e.g. Gd-doped ceria, is capable of generating a giant electromechanical effect that is orders of magnitude larger than other ceramic-based electrostrictors, e.g. lead-based piezoelectrics. This is an unconventional response as it does not obey the Newnham's empirical law and it is atomistically explained by the lability of Ce- pairs. In this report, we investigate the electrostrictive properties of defective ceria with 0.25–3.75% oxygen vacancies introduced by a co-doping

(Sm, Nd) concept. The codoping strategy leads to a different oxygen vacancy configuration in the lattice than for the single dopant case, delineated by a relatively lower vacancy-dopant association energy. This results in electrostrictive response with high strain coefficient (M_{33} in the 0.1-10 10^{-17} m^2/V^2) as well as in marked, strain saturation effects to the applied field from 0 to 120 kV/m and in a relaxation behavior by increasing the frequency of the applied field (0.1 to 1 kHz). Remarkably, M_{33} follows a strict dependency on oxygen vacancy configuration rather than their nominal concentration. Such outcomes define the hypothesis that electrostriction does occur due to oxygen vacancy concentration but it is firmly tuned by oxygen vacancy distribution at the blocking barriers.

4:30 PM

(EMA-S2-027-2020) Intracermic metallic dopant migration leads to formation of lossy crystalline patina in AlN:Mo composites: Mechanisms and insightsR. Grudt^{*1}; S. C. Hayden¹; B. W. Hoff²; M. Hilario²; F. Dynys³; A. E. Baros²; M. Ostraat¹

1. Aramco Services Company, Aramco Research Center – Boston, USA
2. Air Force Research Lab, USA
3. NASA Glenn Research Center, USA

High temperature bulk susceptors and their uses in microwave and mm-wave wireless power transfer applications are of growing utility to the energy community. One material system of interest is a ceramic composite consisting of an aluminum nitride matrix with a molybdenum powder additive. Use of this material system requires a thorough understanding of temperature-dependent electromagnetic and physio-chemical properties. Investigation into the effect of temperature cycling on AlN composites with 0.5 vol% and 3 vol% Mo revealed changes in material dielectric properties and identified new surface phases formed during 10+ temperature cycles up to 1,000 °C in air. The present work focuses on XRD characterization of composite materials, including in situ XRD characterization during heating and identification of new material phases formed during the temperature cycling process. Scanning electron microscopy was employed to identify morphological and compositional changes to the material surface. Identified changes included the formation of both a surface patina by the oxidation of AlN to alumina and a Mo-rich phase in which the Mo became co-located with yttrium, a sintering agent commonly used in AlN manufacturing.

4:45 PM

(EMA-S2-028-2020) Creating Novel Materials through [Ga, Ta] Dipolar-pair Substitution in BaTiO₃ PerovskiteK. Ning^{*1}; H. Shulman¹; S. Tidrow¹

1. Alfred University, Inamori School of Engineering, USA

Dipole-pair substitutions afford a new route for creating diffuse phase transition materials possessing both ferroelectric- and relaxor-like properties that may advance the future design of novel electronic devices. The microstructure, electric and dielectric features of concentration dependent dipole-pair substitutions, [Ga, Ta], for Ti within the perovskite, BaTiO₃, are discussed. The Clausius – Mossotti relation, the new simple material model (NSMM), and, the dipole strength help to explain the unusual properties found in these materials.

S3: Frontiers in Ferroic Oxides: Synthesis, Structure, Properties, and Applications

Ferroelectric Architectures and Devices

Room: Magnolia A

Session Chair: Jiamian Hu, University of Wisconsin-Madison

10:00 AM

(EMA-S3-015-2020) Ultrafast structural dynamics of ferroelectric domains and vortices driven by optical and terahertz fields (Invited)

H. Wen*¹

1. Argonne National Laboratory, X-ray Science Division, USA

Ferroelectrics provide a rich platform to study the dynamics of mesoscale objects such as domains, domain walls, and topological defects. The dimension of these objects is on the order of a few nanometers to micrometers, which poses a characterization challenge to measure their intrinsic structural dynamics. X-ray diffraction imaging following ultrafast excitations enables a direct structural probe of nanoscale dynamical processes associated with domains and vortices. In this talk, I will present the recent progress utilizing ultrafast x-ray techniques to visualize the structural dynamics of ferroelectric domains and vortices driven by optical and terahertz fields. For example, upon optical excitations, ultrafast microdiffraction probe measures light-activated, domain-dependent structural dynamics. Using intense terahertz field as ultrafast electric field control of ferroelectric polarization, we reveal the unique collective motion of ferroelectric polar vortices, as the vortex core oscillates at sub-THz frequencies. These novel dynamics opens opportunities of ultrafast applications utilizing ferroelectric domain and domain walls.

10:30 AM

(EMA-S3-016-2020) Ferroelectric Bloch skyrmion phases induced by structural crystallographic symmetry breaking

J. Hlinka*¹; K. C. Erb¹

1. Academy of Sciences of the Czech Republic, Institute of Physics, Czechia

In this presentation, all 212 Aizu species of structural phase transitions are, for the first time, analyzed with respect to the occurrence of all four possible time-reversal invariant vector and bidirector order parameters and their combinations. It is argued that Bogdanov-Yablonskii phenomenological theory developed earlier for ferromagnetic Bloch skyrmions applies also to the case of ferroelectric Bloch skyrmions. We provide an explicit list of fully ferroelectric and nonferroelastic species of phase transitions, in which the Ginzburg Landau functional allows a polarization gradient invariant of a chiral bidirector symmetry, analogous to the chiral Dzyaloshinskii-Moria term assumed in magnetic Bloch skyrmion theory. We believe that this theoretical analysis will help to discover new types of ferro materials.

10:45 AM

(EMA-S3-017-2020) Microstructure effects on voltage driven ferroelastic domain evolution in polycrystalline $\text{Pb}(\text{Zr}_{0.4}\text{Ti}_{0.6})\text{O}_3$ thin film

K. Yazawa*¹; H. Uchida²; J. Blendell³

1. Purdue University, School of Materials Engineering, USA

2. Sophia University, Japan

3. Purdue University, USA

Ferroelastic domain wall motion is one of the key factors affecting electromechanical coupling. Microstructural effects on ferroelastic domain wall motion are well-known in polycrystalline ferroelectrics. These include factors such as grain size, crystallographic texture and

residual stress. The nature of the grain size effect and residual stress effects on the ferroelastic domain wall motion is addressed. Direct observation of ferroelastic domain wall evolution in thin film PZT with applied DC voltage using piezoelectric force microscopy will be presented. It was demonstrated that the controlling parameter for ferroelastic domain wall motion was the number of colonies of stripe domains in a grain rather than the grain size. Single colony grains did not exhibit out-of-plane (001) domain width change while multiple colony grains showed significant domain width increase with an applied DC voltage. There was no independent grain size effect on ferroelastic domain wall motion in the grain size range (0.5 – 1.5 μm). The ferroelastic switching coercive voltage showed significant fluctuation from grain to grain. A thermodynamic based model of the ferroelastic coercive field with residual normal stresses accurately predicts the coercive voltage fluctuation.

11:00 AM

(EMA-S3-018-2020) Visualizing Strain-Free Domain Walls in Ferroelectrics

S. Mantri*¹; J. Daniels¹

1. UNSW Sydney, Materials Science and Engineering, Australia

A major component of the functionality of ferroelectric materials is due to the domain walls. However, calculating which domain walls are permissible in a symmetry analytically is a complex mathematical problem. With increasing computing resources, we can now calculate the compatibility of the orientation parameter on every plane over the entire spherical orientation space. Comparison of the compatibility can then lead us to the energetically favorable and unfavorable walls. Through this process, not only can we visualize the compatible walls, but can also see how these walls would change as a function of temperature, e.g., 'Strange walls' in orthorhombic ferroelectrics, as a function of changing symmetry, e.g., monoclinic rotation paths like M_A , M_B , and M_C or as a function of electric field. In this paper, we have presented permissible ferroelectric domain walls and their change by analyzing residual strain and charge on all possible planes between orientation states belonging to tetragonal, rhombohedral, orthorhombic and monoclinic symmetry. We have shown how certain walls in orthorhombic do move with temperature and how the monoclinic domain walls move during the transitioning of the ferroelectric from one symmetry to another through various rotation paths.

11:15 AM

(EMA-S3-019-2020) Ferroelectrics for Brain-Inspired Computing (Invited)

Z. Wang¹; A. Khan*¹

1. Georgia Institute of Technology, USA

One of the goals of modern computing as envisioned at its very dawn (i.e., in 1950s) was to mimic the cognitive capabilities of the human being and even to rival them. It is only now that the convergence of machine intelligence and human-like computational capabilities is becoming a realistic proposition--thanks to relentless innovations in computer science as well as underlying hardware platforms, and device and materials engineering. Here, we will show how recent advances in ferroelectric materials can enable computing capabilities akin to those of the functional units of biological brains. We will introduce a ferroelectric neuromorphic platform which can (1) efficiently incorporate both excitatory and inhibitory inputs in an artificial, ferroelectric spiking neuron, and (2) emulate several classes of biological spiking dynamics (such as regular, fast, Thalamo-Cortical spiking and so on). We will discuss the recent experimental demonstrations of ferroelectric spiking neurons and how the rich array of ferroelectric domain dynamics can lead to diverse neuromorphic platforms.

S4: Complex Oxide Thin Film Materials

Discovery: From Synthesis to Strain/Interface Engineered Emergent Properties

Engineered Interface Phenomena I

Room: Orange A

Session Chair: Aiping Chen, Los Alamos National Lab

10:00 AM

(EMA-S4-019-2020) Exploiting interfaces, spin-orbit coupling, and symmetry for novel topological quantum phenomena in oxide heterostructures (*Pioneer in Synthesis*) (Invited)

H. Lee^{*1}

1. Oak Ridge National Lab, USA

Complex oxides are known to possess the full spectrum of fascinating properties. 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 have established a growth technique to control complex oxides at the level of unit cell thickness by pulsed laser epitaxy. The atomic-scale growth control enables to assemble the building blocks to a functional system in a programmable manner, yielding many intriguing physical properties that cannot be found in bulk counterparts. In this talk, examples of artificial and natural oxide superlattices and heterostructures will be presented, highlighting the importance of interface symmetry and spin-orbit coupling. The main topics include topological Hall effects in lattice modulated SrRuO₃ thin films, topologically non-trivial chiral spin textures in SrIrO₃-based heterostructures, and large orbital polarization in infinite-layer nickelate oxides with a square-planar coordination.

10:30 AM

(EMA-S4-020-2020) Interfacial control of chiral magnetic interactions and Hall effect in iridate-manganite superlattices

E. Skoropata^{*1}; J. Nichols¹; J. Ok¹; R. Chopdekar²; E. Choi³; A. Rastogi¹; C. Sohn¹; X. Gao¹; T. Farmer¹; R. Desautels¹; Y. Choi²; D. Haskel²; J. Freeland²; S. Okamoto¹; M. Brahlek¹; H. Lee³

1. Oak Ridge National Laboratory, USA
2. Argonne National Lab, USA
3. Oak Ridge National Lab, USA
4. National High Magnetic Field Laboratory, USA
5. Advanced Light Source, USA

One of the most intriguing outcomes of symmetry breaking and spin-orbit interactions in magnetic systems is the possibility to create non-collinear and chiral spin textures. The Dzyaloshinskii-Moriya interaction (DMI) results from strong spin-orbit coupling and broken inversion symmetry to generate magnetization rotations with fixed chirality. The discovery of magnetic skyrmions originating from DMI in metal films has led to an explosion of efforts to manipulate magnetic phases originating from interfaces. I will describe our progress to understand interface-induced magnetism in epitaxial 3d/5d manganite/iridate superlattices. Our previous work on SrMnO₃/SrIrO₃ superlattices revealed charge-transfer induced interfacial collinear ferromagnetism and an anomalous Hall effect. In LaMnO₃/SrIrO₃ superlattices, we find a large additional topological Hall effect arising from the interaction of charge carriers with a noncoplanar chiral spin texture induced by DMI. I will describe how the interfacial atomic layer stacking and symmetry enabled by the nonmagnetic A-sites determine the competition between interfacial collinear and chiral magnetic interactions. Bulk and interface

electronic and magnetic properties from magnetometry measurements, soft, and hard x-ray experiments will be compared to provide insight to the atomic-scale control of DMI at oxide interfaces.

10:45 AM

(EMA-S4-021-2020) Mapping phase stability of the metallic delafossite PdCrO₂ using pulsed laser deposition

J. Ok^{*1}; H. Lee¹

1. Oak Ridge National Lab, USA

PdCrO₂ is one of the rare metallic triangular-lattice antiferromagnets in the ultraclean limit. Here, we report successful growth of the metallic delafossite PdCrO₂ film by pulsed laser deposition (PLD). We have systematically mapped the growth of PdCrO₂ across growth temperature (T), oxygen partial pressures (P_{O₂}), laser fluences (E) and across many substrate types. It is found that the formation of PdCrO₂ is extremely sensitive to growth conditions as well as epitaxial strain and the chemical and structural character of the substrate. Our film grown at optimized condition is fully metallic, has narrow rocking curve width (0.103°), and exhibits magnetic behavior with antiferromagnetic transition at T_N ~ 37 K, consistent with the bulk crystal.

11:00 AM

(EMA-S4-022-2020) Polarization induced strain vs. charge mediated magnetoelectric coupling across the PZT/LSMO interfaces

B. Paudel^{*1}; I. Vasiliev¹; M. Hammouri²; D. Karpov³; A. Chen⁴; V. Lauter⁵; E. Fohntung⁶

1. New Mexico State University, Physics, USA
2. California State University, Los Angeles, USA
3. Paul Scherrer Institute, Switzerland
4. Los Alamos National Lab, USA
5. Oak Ridge National Lab, USA
6. Rensselaer Polytechnic Institute, USA

We study magnetoelectric coupling at the interface of a ferroelectric PbZr_{0.2}Ti_{0.8}O₃ (PZT) and magnetic La_{0.67}Sr_{0.33}MnO₃ (LSMO) heterostructure utilizing polarized neutron reflectometry (PNR) and density functional theory (DFT) calculations by applying electric field, which switches polarization direction of PZT layer. PNR results show that PZT/LSMO interface undergoes ferromagnetic (FM) to A-antiferromagnetic (A-AF) phase transition due to hole accumulation on LSMO for polarization direction away from interface and retains its FM phase despite of hole depletion when polarization points towards the interface. The global magnetization of LSMO also changes by switching polarization direction and changing the strength of electric field. DFT calculations indicate that enhanced magnetization correlates with an out of plane tensile strain, whereas the suppressed magnetization is attributed to out of plane compressive strain and show the coexistence of FM and A-AF phases even at zero out of plane strain. Charge modulations throughout the LSMO layer appear to be unaffected by strain, suggesting that these modulations do not significantly change the global magnetization. PNR and DFT results are in consort to verify that the interfacial magnetic modulations are due to co-action of strain and charge mediated effects with strain and charge effects dominant at different length scales.

11:15 AM

(EMA-S4-023-2020) Chemistry and Strain Mediated Magnetism in Ultra-thin LSMO-LSCO Heterostructures

A. N. Penn^{*1}; S. Koohfar²; D. P. Kumah²; J. M. LeBeau³

1. North Carolina State University, Materials Science and Engineering, USA
2. North Carolina State University, Physics, USA
3. Massachusetts Institute of Technology, Materials Science and Engineering, USA

Atomic-scale interactions between structurally similar but chemically different materials at epitaxial interfaces provide a route to control the electronic and magnetic properties of ultra-thin materials. $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) is a model system where deviations in stoichiometry and atomic-scale structural distortions induced at LSMO heterointerfaces can lead to magnetic and metal-insulator transitions. Contributing factors include electronic and atomic reconstructions that occur at the interface between LSMO film and substrate due to the polar discontinuity when grown on SrTiO_3 . Isovalent spacer layers of $\text{La}_{0.7}\text{Sr}_{0.3}\text{CrO}_3$ (LSCO) are inserted to mitigate the polar discontinuity and have shown to produce ultra-thin LSMO films that maintain their magnetic character. To understand the microscopic origin for the stabilization of magnetism, we report an investigation of LSMO/LSCO multilayer thin films using scanning transmission electron microscopy. A variation in the out-of-plane lattice parameters with each layer, accompanied by a 5% inhomogeneity in the La/Sr ratio and Mn/Cr intermixing are determined using atomic resolution imaging and energy dispersive x-ray spectroscopy. Additionally, electron energy-loss spectroscopy indicates an accumulation of oxygen vacancies in the interlayers. This investigation highlights the large-scale impact of subtle chemical variations in heterostructured thin films.

11:30 AM

(EMA-S4-024-2020) Ferromagnetism in Strained Epitaxial LaCoO_3

S. Yoon^{*1}; X. Gao¹; J. Ok¹; Z. Liao¹; M. Han²; P. Ganesh³; W. Choi⁴; H. Lee¹

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Brookhaven National Laboratory, Condensed Matter Physics and Materials Science Department, USA
3. Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, USA
4. SungKyunKwan University, Physics, Republic of Korea

Since the initial report on the ferromagnetism with $T_c \approx 90\text{K}$ in tensile-strained epitaxial LaCoO_3 (LCO) films as opposed to the nonmagnet ground state found in bulk materials, a number of experimental and theoretical studies have been carried out over the past decade. As a result, a wealth of knowledge about epitaxial LCO films has been accumulated, and several mechanisms have been proposed, including ferroelasticity, oxygen vacancy ordering, octahedral tilt, and spin state ordering. Previously, we observed unusual structural modulations, consisting of dark lines and bright regions in tensile-strained LCO films and proposed that dark lines seen in STEM images are associated with the emergent ferromagnetic property. Herein, using more advanced STEM imaging techniques with a higher precision, we revisited epitaxial LCO films grown on SrTiO_3 substrates. We found monoclinic-like and orthorhombic-like unit cells, and the monoclinic-like unit cells always coexisted along the dark lines with two unit cell thickness. This result indicates that the two-unit-cell-thickness monoclinic domain is also another unique structure strongly coupled to the dark line in the tensile-strained LCO films. Finally, we will discuss the possibility that the rock-salt type high-spin/low-spin state ordering, strongly suggested by recent x-ray diffraction experiments, is stabilized in this monoclinic domain region.

11:45 AM

(EMA-S4-025-2020) Electronic structure and defect interactions at $\text{LaMnO}_3/\text{SrTiO}_3$ polar/non-polar heterojunctions (Invited)

T. Kaspar^{*1}; P. Sushko²; M. Bowden³; D. Keavney⁴; M. Sassi¹; S. R. Spurgeon⁵; S. Chambers⁶

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
2. Pacific Northwest National Lab, Physical Sciences Division, USA
3. Pacific Northwest National Lab, EMSL, USA
4. Argonne National Lab, Advanced Photon Source, USA
5. Pacific Northwest National Laboratory, Energy and Environment Directorate, USA
6. Pacific Northwest National Laboratory, Physical Sciences Division, USA

The deposition of polar perovskites on non-polar substrates has been predicted to lead to a increasing electric field in the film that increases continuously as the film thickness increases; this is known as the polar catastrophe. Polar perovskites (ABO_3) in which the B-site cation is a transition metal capable of adopting multiple oxidation states can take one of several pathways to alleviate this polar catastrophe. We use epitaxial $\text{LaMnO}_3(001)/\text{SrTiO}_3(001)$ heterojunctions as a model system to explore these pathways. Using x-ray photoelectron spectroscopy, Mn L-edge x-ray absorption spectroscopy, and spatially resolved electron energy loss spectra in scanning transmission electron microscopy images, we elucidate the electronic structure and interfacial band alignment of the heterojunction. Correlation with density functional theory calculations allows us to develop a model for the behavior of polar/nonpolar $\text{LaMnO}_3(001)/\text{SrTiO}_3(001)$ heterojunctions in which the polar catastrophe is alleviated by the formation of oxygen vacancies at the LaMnO_3 surface. We then explore the interaction of point defects at the heterojunction interface by irradiating with 1 MeV Zr^+ ions. Differences in defect interactions and damage behavior between polar (001)-oriented and non-polar (111)-oriented heterojunctions reveal the effect of the polar discontinuity.

Engineered Interface Phenomena II

Room: Orange A

Session Chair: George Kotsonis, The Pennsylvania State University

2:00 PM

(EMA-S4-026-2020) Band-gap engineering, charge transfer and built-in electric fields across semiconductor-crystalline oxide interfaces (Invited)

J. Ngai^{*1}

1. University of Texas-Arlington, Physics, USA

The control of band-alignment, charge transfer and built-in electric fields across interfaces between semiconductors underpins the functionality of virtually all semiconducting devices, ranging from solar cells to transistors. Advances in thin-film epitaxy now enable such engineering principles to be explored across interfaces comprised of semiconductors and multifunctional oxides. Here, we discuss how composition can be manipulated to alter band-alignment, as well as induce charge transfer and the formation of built-in electric fields in two archetype systems, namely, $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$ on Ge and $\text{SrNb}_x\text{Ti}_{1-x}\text{O}_3$ on Si, respectively. For $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$ on Ge, current-voltage, capacitance-voltage and photoemission spectroscopy measurements reveal how band-alignment can be altered from type-II to type-I with Zr content. For $\text{SrNb}_x\text{Ti}_{1-x}\text{O}_3$ / Si heterojunctions magneto-transport measurements indicate the formation of a hole gas in the Si as Nb content in the oxide is varied. Core-level spectra obtained through hard x-ray photoelectron spectroscopy reveal striking asymmetries that allow us to map band-bending across the $\text{SrNb}_x\text{Ti}_{1-x}\text{O}_3$ / Si heterojunction. Tuning of both band-alignment and charge density within a single heterojunction could enable the functionality of semiconductor-oxide heterojunctions to be engineered, akin to heterojunctions comprised of III-V semiconductors.

2:30 PM

(EMA-S4-027-2020) Confinement-driven magnetism in SrTiO₃ quantum well heterostructuresR. F. Need^{*1}; P. Marshall²; B. Isaac²; B. Kirby³; J. Borchers³; A. Suter⁴; S. Stemmer²; S. D. Wilson²

1. University of Florida, Materials Science & Engineering, USA
2. University of California, Santa Barbara, Materials, USA
3. National Institute of Standards and Technology, USA
4. Paul Scherrer Institut, Switzerland

Through heterostructure design, we generate emergent magnetic behavior in SrTiO₃ quantum wells embedded within Mott insulating rare earth titanate RTiO₃ (R = Gd, Sm) matrices. At the RTiO₃/SrTiO₃ interface, a conduction band offset leads to charge transfer and forms a high-density, strongly-correlated two-dimensional electron liquid (2DEL) that resides within the SrTiO₃. By changing the SrTiO₃ layer thickness, we tune the three-dimensional carrier density and magnetic exchange interactions of the 2DEL electrons. A combination of polarized neutron reflectometry and low-energy muon spin rotation was used to probe the magnetism in the buried SrTiO₃ layers as a function of well thickness and barrier composition. Our results show that there is a critical well thickness of ~2 nm, below which the 2DEL electrons exhibit robust magnetic correlations. The critical thickness is independent of the neighboring layer chosen; however, the sign of the 2DEL's magnetic exchange interactions follow that of the host matrix. In other words, SrTiO₃ electrons within a ferrimagnetic GdTlO₃ matrix display ferromagnetic behavior, while SrTiO₃ electrons embedded within antiferromagnetic SmTiO₃ exhibit antiferromagnetic correlations. Together, this work highlights the how the interplay between charge transfer, quantum confinement, and magnetic proximity can engender emergent phase behavior in strongly correlated systems.

2:45 PM

(EMA-S4-028-2020) Structural analysis of the polar – nonpolar LaInO₃/BaSnO₃ perovskite oxides interfaceM. Zupancic^{*1}; T. Markurt¹; W. Aggoune²; K. Char³; Y. Kim³; Y. Kim³; C. Draxl²; M. Albrecht¹

1. Leibniz-Institut für Kristallzüchtung, Materials Science (Electron Microscopy), Germany
2. Institute of Physics, Humboldt University of Berlin, Germany
3. Institute of Applied Physics, Seoul National University, Dept. of Physics and Astronomy, Republic of Korea

Two-dimensional electron gases (2DEG) formed at the interface between polar and nonpolar oxides attracted considerable attention in the last decade. In case of the archetypical interface between SrTiO₃ (STO) and LaAlO₃ (LAO) the 2DEG is attributed to the charge discontinuity and the charge transfer of electrons from the polar LAO to the nonpolar STO. Yet, its origin is still debated. Recently, the interface between cubic perovskite BaSnO₃ (BSO) and orthorhombic LaInO₃ (LIO) attracted attention due to the high electron mobility of ~300cm²/Vs in BaSnO₃ at room temperature. Here, we combine TEM techniques and first principle calculations to study the origin of the 2DEG at the BSO/LIO interface. We focus on the role of the octahedral tilt at BSO/LIO interface and the BSO surface termination. Our study reveals that the octahedral tilt increases gradually from a cubic BSO (no tilt) to the bulk value of LIO along few pseudo cubic unit cells. In parallel, the out-of-plane lattice parameter of the LIO layer increases within these few unit cells. We hypothesize that the octahedral tilt suppression at the interface causes an interfacial polarization that significantly contributes to confining the 2DEG at the interface. Since ab-initio studies show that BSO termination at the interface is decisive in the 2DEG formation, we study both, a cleaved BSO surface and the interface after growth of the LIO film.

3:00 PM

(EMA-S4-029-2020) Oxide Heterostructures Integrated with Si(100) (Invited)S. Singamaneni^{*1}

1. The University of Texas at El Paso, USA

Multifunctional heterostructures can exhibit a wide range of functional properties, including colossal magneto-resistance, magnetocaloric, and multiferroic behavior, and can display interesting physical phenomena including spin and charge ordering and strong spin-orbit coupling. Most of these oxides were epitaxially deposited on lattice matching substrates such as SrTiO₃. However, putting this functionality to work remains a challenge in microelectronics industry. This presentation discusses recent advances in the integration and investigation of the properties of complex magnetic (La_{0.7}Sr_{0.3}MnO₃; SrRuO₃) and ferroelectric oxides (BiFeO₃ and BaTiO₃) onto silicon substrates. The opportunities and challenges will be outlined.

Machine Learning Driven Synthesis

Room: Orange A

Session Chairs: Elizabeth Paisley, Sandia National Laboratories; Kevin Ferri, North Carolina State University

4:00 PM

(EMA-S4-030-2020) Combinatorial Experimentation and Machine Learning for Materials Discovery (Pioneer in Synthesis) (Invited)I. Takeuchi^{*1}

1. University of Maryland, USA

We have developed combinatorial thin film synthesis and characterization techniques in order to perform rapid survey of previously unexplored materials phase space in search of new inorganic functional materials with enhanced physical properties. For oxide thin films, we use combinatorial pulsed laser deposition. Over the years, the challenges in the high-throughput approach has evolved from synthesis of large number of disparate compounds to developing quantitatively accurate rapid characterization tools to analysis and digestion of large amount of data churned out by the methodology. To address the last challenge, we are increasingly relying on machine learning techniques including pattern recognition within diffraction data to construct phase diagrams and mining experimental databases to look for trends in materials properties for future predictions. I will also discuss our latest effort where active learning is used to design and steer the sequence of experiments in order to maximize attainable knowledge, minimize experimental resources, and as a result further speed up the materials discovery process. This work is performed in collaboration with A. Gilad Kusne, V. Stanev, A. Mehta, B. DeCost, and J. Hattrick-Simpers. This work was funded by ONR, DOE, and NIST.

4:30 PM

(EMA-S4-031-2020) Fabrication and characterization of epitaxial Li-oxide thin films and devices for neuromorphic computingH. Yu^{*1}; J. Pearson¹; Y. Gong¹; Y. Ren¹; I. Takeuchi²

1. University of Maryland, College Park, Department of Materials Science and Engineering, USA
2. University of Maryland, USA

We are performing a systematic investigation of the multi-level switching operation in the Li-ion synaptic devices based on epitaxial Li_{1-x}CoO₂ (LCO) thin films with different dimensions and orientations. These epitaxial films were fabricated on (100), (110), and (111) SrTiO₃ (STO) substrates at 700 °C utilizing the pulsed laser

deposition method. Through the Li-ion exchange between the electrolyte and the LCO channel, non-volatile multi-level resistive states can be established by applying the current or voltage pulses with different duration or amplitudes. The switching speed and energy consumption exhibit lattice-orientation dependence of the LCO channel, indicating that the anisotropy of the Li-ion diffusion rate along different LCO crystal planes plays an important role in device performance. Comparing the devices with different thickness LCO channels, we find that reducing the thickness of the LCO channel can substantially improve the signal-to-noise ratio of the non-volatile switching. Also, epitaxial Nb-doped $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) thin films which are considered to be an ideal solid-state electrolyte, was successfully fabricated on $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ (GGG) substrates with different orientations at 700 °C by pulsed laser deposition. Electrochemical measurements are ongoing. This project is funded by ONR.

4:45 PM

(EMA-S4-032-2020) A Data-Driven Approach to Guiding Synthesis of Oxides (Invited)

P. Balachandran*¹

1. University of Virginia, Materials Science and Engineering, USA

One of the challenges in the use of computational methods to accelerate the search and discovery of new materials is the lack of guidelines to predict their stability or formability, especially when the complexities of the materials grow in terms of chemistry, dimensionality and stoichiometry. Although the convex hull method that leverages the total energy data from density functional theory (DFT) calculations provide valuable insights, such approaches are limited by the capabilities of the DFT methods. Alternatively, data-driven methods built on the foundations of machine learning (ML) can guide experiments towards promising regions in the design space. However, these methods rely on available data to train the statistical models which present new challenges in the form of having to deal with small, imbalanced, and heterogeneous data. In this talk, I will review our past research where we have demonstrated the potential of ML methods to predict formable new complex oxides. In addition, I will also discuss some of our on-going efforts on the application of ML methods for more complex materials such as the high entropy oxides.

S6: Complex Oxide and Chalcogenide Semiconductors: Research and Applications

Design and Discovery of Complex-Structured Semiconductors

Room: Magnolia A

Session Chairs: Rafael Jaramillo, Massachusetts Institute of Technology; Jian Shi, Rensselaer Polytechnic Institute

2:00 PM

(EMA-S6-001-2020) Combinatorial Approach to Chalcogenide Thin Films (Invited)

I. Takeuchi*¹

1. University of Maryland, USA

We are using the composition spread technique to explore novel functional chalcogenide materials. Co-sputtering is used to synthesize composition spreads of selenides and tellurides in a high vacuum chamber. We have demonstrated fabrication of low loss integrated photonic switch using our $\text{Ge}_2\text{Sb}_2\text{Te}_5$ thin films. We are carrying out mapping of properties of various ternary systems such as Ge-Sb-Te and Ti-Sb-Te as phase change materials (PCMs). We are using machine learning to rapidly analyze the data and in particular active learning using the Bayesian approach to quickly determine the structural phase diagram with minimum number of

characterization experiments. In the Ge-Sb-Te, we have identified a new composition where the PCM figure of merit (Dn/k) is up to a factor of 3 larger than that of the 225 compound on the same spread. Origin of the enhanced properties will be discussed. Investigation and mapping of superconductivity in Fe-Se-Te will also be discussed. This project is performed in collaboration with Heshan Yu, A. Gilad Kusne, Mo Li, and it is funded by an ONR MURI and NIST.

2:30 PM

(EMA-S6-002-2020) Understanding the Surface of Epitaxial SrTiO_3 Films Grown by Hybrid MBE

S. Thapa*¹; S. R. Provence¹; M. Brahlek²; L. Jason²; W. Jin¹; R. B. Comes³

1. Auburn University, Dept. of Physics, USA

2. Oak Ridge National Lab, USA

3. Auburn University, Dept. of Physics, USA

Hybrid oxide molecular beam epitaxy (hMBE), where transition metal cations are delivered using a metal-organic precursor, has emerged as the state-of-the-art approach to the synthesis of electronic-grade complex oxide films. However, numerous questions remain regarding the mechanism of the growth process and the surface properties of the resulting films. To examine these properties, thin film SrTiO_3 (STO) was prepared by hMBE using a titanium tetraisopropoxide (TTIP) precursor for Ti delivery and an elemental Sr source on annealed STO substrates with varying Ti:Sr flux ratios to examine the conditions for the reported stoichiometric growth window. Principle component analysis of RHEED images acquired during growth is used to understand the surface evolution. In vaco XPS analysis post-growth enabled understanding the surface elemental composition in the STO samples. Low energy electron microscopy measurements were also performed to correlate the XPS data with the surface termination. To compare the surface sensitive results with previously reported bulk measurements, samples were also examined using x-ray diffraction to compare our results with the literature [BM1]. These studies explain the mechanisms of hMBE growth and the resulting surface structure of films grown within the MBE growth window. Such results can open new opportunities for the study of interfacial structures synthesized via hMBE.

2:45 PM

(EMA-S6-003-2020) Structural and Electronic Characterization of Epitaxial $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$ Spinel Films

M. Blanchet*⁴; A. C. Bredar¹; W. Bowers⁴; S. Chikara²; T. Kaspar³; S. Heald³; B. Farnum¹; R. B. Comes⁴

1. Auburn University, Dept. of Chemistry, USA

2. Florida State University, National High Magnetic Field Laboratory, USA

3. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA

4. Auburn University, Dept. of Physics, USA

Investigations of spinel materials have shown many of them to exhibit strong catalytic behavior through oxygen reduction reactivity, indicating their future application in water splitting and fuel cell technology. Despite this, limited work has been done in characterizing their structural and electronic properties, and even less work has been done in examining them as epitaxial thin films. To further this field of study, $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$ spinel thin films were synthesized and characterized using a variety of experimental methods. Films were grown using molecular beam epitaxy, and samples of varying composition were incorporated to identify links between their cation stoichiometry and properties. Of note are conclusions made of this spinel's cation valence and lattice site coordination using in-situ x-ray photoelectron spectroscopy and K-edge x-ray absorption spectroscopy. We also include our results from x-ray diffraction, ellipsometry and scanning transmission electron microscopy. This research provides characterization knowledge important for this material's future application as an inexpensive oxygen reduction reaction catalyst.

3:00 PM

(EMA-S6-004-2020) Optical properties, dielectric screening, and heterojunction design for oxides and chalcogenides (Invited)A. Schleife*¹

1. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA

High-performance computing enables quantum-mechanical studies of material properties with unprecedented accuracy: Many-body perturbation theory predicts electronic and optical properties in excellent agreement with experiment. Modern materials databases allow searching for optimal candidates, potentially without any or minimal additional experiments or simulations. I will illustrate how the GW+BSE approach allows studying the impact of dielectric screening contributions on optical and excitonic properties of oxides and chalcogenides and will disentangle the influence of free carriers, electronic screening, and lattice polarizability. The resulting optical-absorption spectra provide insight into the dominating physics and allow us to unequivocally distinguish crystal phase in CdSe semiconductor nanocrystals and bulk ZnO, based on optical properties. While first-principles simulations provide deep insight and allow for predictive accuracy, they require significant computational resources. I will also describe how incorporating information from first-principles simulations that is collected in large, freely available online databases into computational research on excited electronic states can side-step the problem of high computational cost. To this end, we used Materials Project and branch-point energy alignment to facilitate efficient design of semiconductor heterojunctions.

4:00 PM

(EMA-S6-005-2020) Computational discovery of ambipolarly doped ultra-wide-band-gap oxide and high-entropy chalcogenide semiconductors (Invited)E. Kioupakis*¹

1. University of Michigan, Materials Science and Engineering, USA

In this talk I will present result from predictive atomistic calculation on the computational discovery of new oxide and chalcogenide semiconducting materials. Ultra-wide-band-gap (UWBG) semiconductors, with gaps wider than the 3.5 eV gap of GaN, have tremendous potential to advance power-electronic devices, but ambipolar doping has been a major challenge. Using hybrid density functional theory, we demonstrate rutile germanium oxide to be an alternative UWBG (4.68 eV) semiconductor that can be ambipolarly doped. We also propose a new class of semiconducting materials based on high-entropy chalcogenides. By combining high-throughput first-principles calculations with experimental synthesis and characterization, we show that GeSnPbSSeTe is thermodynamically stable over the competing binary phases and exhibits ambipolar dopability. Our work demonstrates the potential of entropy stabilization in the discovery of novel semiconductors. This work was performed in collaboration with Sieun Chae, Kelsey Mengle, Jihang Lee, Zihao Deng, Logan Williams, Guangsha Shi, John Heron, Alan Olvera, Juan Lopez, Joseph Casamento, Ruiming Lu, and Ferdinand Poudeu. It was supported by the National Science Foundation under grant numbers 1534221 and 1561008. Computational resources were provided by the DOE NERSC facility.

4:30 PM

(EMA-S6-006-2020) Modulation Doping in Alkaline-Earth Stannates (Invited)B. Jalan*¹

1. University of Minnesota, USA

Interfaces between perovskite oxides have created tremendous excitement because of the potential for emergent phenomena and novel field-effect devices. The vast majority of these papers focus on the LaAlO₃/SrTiO₃ (LAO/STO) interfaces including some on Al₂O₃/STO and ReTiO₃/STO (Re refers to the rare-earth elements)

interfaces among others. Amazingly, all these heterostructures involve the use of STO as an active layer where electron transport occurs. Attempts to synthesize non-STO based modulation-doped heterostructure have been unsuccessful so far despite theoretical predictions. Nor has any appreciable level of control been gained over the electron density at the interface. Here, we will report the first demonstration of true modulation doping in a wider bandgap perovskite oxide without the use of STO. We show that the La-doped SrSnO₃/BaSnO₃ precisely fulfills the theoretical criteria for electron doping in BaSnO₃ using electrons from La-doped SrSnO₃, and we demonstrate how rearrangement of electrons can be used to control the insulator-to-metal transition in these heterostructure. We further show the use of angle-resolved HAXPES as a non-destructive approach to not only determine the location of electrons at the interface but also to quantify the width of electron distribution in BaSnO₃. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

5:00 PM

(EMA-S6-007-2020) Opportunities in epitaxial mixed-anion oxyfluoride perovskites (Invited)S. May*¹

1. Drexel University, Materials Science and Engineering, USA

The ability to carry out topochemical reactions on epitaxial complex oxide films is an enabling strategy for expanding the accessible chemistries in oxide heterostructures. In this talk, I will describe how post-deposition fluorination processes can yield both uniform and laterally-patterned oxyfluoride perovskites. Using recent work on SrMnO_{2.5-δ}F_γ as an example, I will discuss the fluorination reaction used to incorporate fluorine into as-grown perovskite oxide films. Epitaxial strain is found to influence both the amount of F incorporated within SrMnO_{2.5-δ}F_γ and the anion site occupied by F. The resultant physical properties of the electron-doped manganite oxyfluoride will be discussed, highlighting the contrast in electronic, magnetic, and optical behavior obtained through anion substitution as compared to A-site substituted La_{1-x}Ce_xMnO₃. In the second half of the talk, I'll present how topochemical reactions can be spatially controlled through lithographically-defined hard masks, allowing for the realization of in-plane SrFeO_{2.5}/SrFeO₃ and SrFeO_{2.5}/SrFeO₂F superlattices. These lateral heterostructures exhibit many features distinct from traditional patterned materials such as tunable anisotropy, non-binary properties, and reconfigurability, offering the potential for dynamic control over lateral patterns. This work was supported by the National Science Foundation (NSF), grant number CMMI-1562223.

S7: Superconducting and Magnetic Materials: From Basic Science to Applications**Superconducting and Magnetic Materials I**

Room: Cypress B

Session Chair: Xingjiang Zhou, National Lab for Superconductivity

2:00 PM

(EMA-S7-001-2020) New materials research and functional development of perovskite-related osmium oxide (Invited)K. Yamaura*¹

1. National Institute for Materials Science, Japan

High-pressure synthesis and crystal growth of solid-state osmium oxides, which are perovskite-related, and their magnetic and electrical properties will briefly be reviewed. A new polymorph of the triple perovskite Ba₃CuOs₂O₉, which usually exists in the orthorhombic phase, was synthesized under high-pressure and high-temperature conditions at 6 GPa and 1100 °C. Under the

synthetic condition, $\text{Ba}_3\text{CuOs}_2\text{O}_9$ crystallizes into a hexagonal structure ($P6_3/mmc$) and undergoes a 1.36% increment in density, compared to that of the orthorhombic phase. Although $\text{Ba}_3\text{CuOs}_2\text{O}_9$ maintains its 6H perovskite-type structure, the distribution of Cu and Os atoms are dramatically altered. The hexagonal $\text{Ba}_3\text{CuOs}_2\text{O}_9$ exhibits a ferrimagnetic transition at 290 K, which is in stark contrast to the antiferromagnetic transition at 47 K exhibited by the orthorhombic $\text{Ba}_3\text{CuOs}_2\text{O}_9$. The enhanced transition temperature is most likely due to the strongly antiferromagnetic $\text{Os}^{5+}-\text{O}-\text{Os}^{5+}$ bonds and the moderately antiferromagnetic $\text{Os}^{5+}-\text{O}-\text{Cu}^{2+}$ bonds, the angles of which are both approximately 180° . The 290 K ferrimagnetic transition temperature is the highest reported for triple-perovskite osmium oxides. Besides, the coercive field is greater than 70 kOe at 5 K, which is remarkable among the coercive fields of magnetic oxides.

2:30 PM

(EMA-S7-002-2020) Quantum effects of a layered perovskite with triangular-lattice (Invited)

J. Ma^{*1}; H. Zhou²; y. Kamiya¹

1. Shanghai Jiao Tong University, China
2. University of Tennessee, USA

Investigating the exotic quantum phenomena and the related ground state of the frustrated quantum magnets has caught a lot of attention, and the exotic phases has been recognized by modifying the relationship between the spin, orbital, and lattice degrees of freedom. The two-dimensional Spin-1/2 triangular-lattice antiferromagnet (TLAF) is a typical example. The effect of the quantum fluctuations in the system could interfere the spin states, such as the disordered liquid and glass phases, and keep them with the complicated interactions among the geometric frustration, low dimensionality, and small spin. $\text{Ba}_3\text{CoSb}_2\text{O}_9$ is the first spin-1/2 equilateral TLAF vanishing Dzyaloshinskii-Moriya. The magnetic Co^{2+} layers are well separated by the non-magnetic clusters of the Sb_2O_9 biotahedra and Ba^{2+} ions. With the help of the magnetic susceptibility, heat capacity, elastic and inelastic neutron scattering techniques, the strong quantum effects were observed from a non-collinear 120° spin structure in zero magnetic field into a collinear up-up-down state in a finite range of applied magnetic field. Through detailed comparisons with the linear/nonlinear spin-wave theories and the effect of interlayer interaction, we point out that the large-S approximation is inadequate to explain our experimental observation. Moreover, we have extended the work to the other TLAFs of the layer-perovskite compounds with $S=1$ and $5/2$.

3:00 PM

(EMA-S7-003-2020) Intrinsic 2D Topological Materials: Spin-orbit Spillage, Properties, and Calculation Reliability

K. Choudhary^{*1}

1. National Institute of Standards and Technology, MML, USA

Two-dimensional materials have shown ubiquitous properties which cannot be found in the 3D counterparts. Using density functional theory-based spin-orbit spillage, Wannier-interpolations and allied calculations we identify several metallic, semiconducting, magnetic and non-magnetic topologically non-trivial intrinsic 2D materials. Using JARVIS-DFT 2D material dataset we first identify materials with high spin-orbit spillage among 683 materials resulting in 108 materials with high-spillage values. Then we use Wannier-interpolation to carry-out Z₂, Chern-number, anomalous hall conductivity, Curie temperature surface and edge state calculations to identify topological insulators and semimetals such as QSHI, QAHI, magnetic and non-magnetic semimetals. For a subset of predicted QAHI materials, we run GW+SOC and GGA+U calculations. We find that as we introduce many-body effects only few materials retain non-trivial band-topology suggesting the importance of high-level DFT methods in predicating 2D topological

materials. However, as an initial step, the automated spillage screening and Wannier-approach provide excellent predictions for finding new topological materials.

3:15 PM

(EMA-S7-004-2020) Machine Learning of the Functional Form of the Superconducting Critical Temperature

S. R. Xie¹; G. R. Stewart²; J. J. Hamlin²; P. J. Hirschfeld²; R. G. Hennig^{*1}

1. University of Florida, Materials Science and Engineering, USA
2. University of Florida, Physics, USA

Predicting the critical temperature T_c of superconductors is a notoriously difficult task, even for electron-phonon systems. We build on earlier efforts by McMillan and Allen and Dynes to model T_c from various measures of the phonon spectrum and the electron-phonon interaction by using machine learning algorithms. Specifically, we use the Sure Independence and Sparsifying Operator (SISSO) method to identify a new, physically interpretable equation for T_c as a function of a small number of physical quantities. We show that our model, trained using the relatively small $T_c < 10\text{K}$ data tested by Allen and Dynes, improves upon the Allen-Dynes fit and can reasonably generalize to superconducting materials with higher T_c such as H₃S. By incorporating physical insights and constraints into a data-driven approach, we demonstrate that machine-learning methods can identify the relevant physical quantities and obtain predictive equations using small but high-quality datasets.

Superconducting and Magnetic Materials II

Room: Cypress B

Session Chair: Kazunari Yamaura, National Institute for Materials Science

4:00 PM

(EMA-S7-005-2020) Non-Fermi Liquid Behaviors, Nodal Superconducting Gap and Insulating Parent Phase in Iron-Based Superconductors (Invited)

X. Zhou^{*1}

1. Institute of Physics, National Lab for Superconductivity, China

We have studied electronic structure of iron-based superconductors by high-resolution angle-resolved photoemission spectroscopy. In this talk, I will introduce three of our recent work. (1). Emergence of superconductivity from fully incoherent normal state in optimally-doped $(\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2$ superconductor ($T_c \sim 38\text{K}$) [1]. We find that, while sharp superconducting coherence peaks emerge in the superconducting state on the hole-like Fermi surface sheets around the zone center, no quasiparticle peak is present in the normal state. Its electronic behaviors deviate strongly from a Fermi liquid system; (2). Orbital origin of robust nodal superconducting gap in the nematic state of bulk FeSe superconductor ($T_c = 8 \sim 9\text{K}$) [2]. We also reveal multiple and highly anisotropic hole-like Fermi surface sheets and nodal superconducting gap in the nematic state of the FeSe superconductor that are robust against nematic domains and disorder [3]; (3). We find that the parent phase of the single-layer FeSe/SrTiO₃ films is insulating, and its doping evolution is very similar to doping a Mott insulator in cuprate superconductors [4].

4:30 PM

(EMA-S7-006-2020) Using atomic forces to understand and manipulate unconventional superconductors (Invited)

P. Maksymovych^{*1}

1. Oak Ridge National Laboratory, USA

Atomically sharp tip can apply up to several nN of force to single adsorbed and embedded atoms. Precise measurements of atomic forces and their inhomogeneity enable identification of atomic

lattices, point and long-range defects, often with superior resolution and sensitivity compared with more common tunneling microscopy. To this end, I will first illustrate a rich pattern of as-grown lattice defects, including point vacancies and extended dislocations and their effect local electronic structure of Co-doped BaFeAs superconductor, revealed with combined force and tunneling microscopy. Subsequently, I will discuss reproducible injection of a variety of defects into the otherwise atomically pristine surface of FeSe. Intriguingly, the force microscopy revealed the propensity to counterintuitive sub-surface defect formation. Finally, I will present the use of multivariate data analytics techniques to construct local structure-function libraries connecting characteristic electronic states and electron-hole asymmetry to intrinsic and introduced lattice defects. Going forward, local control over surfaces and edge-terminations enables new insight into confinement effects on superconductivity, as well as disorder and edge states in topological superconductors. Research carried out at the Center for Nanophase Materials Sciences in Oak Ridge National Lab, which is a DOE Office of Science user facility.

5:00 PM

(EMA-S7-007-2020) Miscibility gap and intrinsic anti-ferromagnetic Griffith phase in $\text{Sr}(\text{Fe}_{1-x}\text{Mn}_x)_2\text{As}_2$ phase diagram with multi-critical points

G. Wang^{*1}; L. Chen¹; C. Cao¹; H. Chen¹; J. Ma²; J. Hu¹; X. Chen¹

1. Institute of Physics, Chinese Academy of Sciences, China
2. Shanghai Jiao Tong University, China

The crystal structure, magnetic and electronic properties of Mn-doped SrFe_2As_2 single crystals have been systematically investigated. A miscibility gap is found in the system from $x \sim 0.4362(4)$ to $x \sim 0.9612(9)$, and out of the gap single crystals hold two distinct structures, $I4/mmm$ (139) for Fe-rich side and $P-3m1$ (164) for Mn-rich side, respectively. For Fe-rich side, single crystals have a continuously enlarged lattice parameter c for $x < 0.2055(2)$, followed by a phase separation with the crystals holding different structures up to $x = 0.4362(4)$. Magnetic and electronic transportation measurements demonstrate the suppression of spin density wave from $x = 0$ to $x = 0.0973(1)$ and the following abnormal increase of the ordering temperature, which is attributed to the intrinsic anti-ferromagnetic Griffith phase [1, 2]. The heat capacity further confirms these novel phenomena. Finally, a phase diagram with multi-critical points covering the whole composition range of Mn-doped SrFe_2As_2 system is established accordingly. [1] R.B. Griffiths, Nonanalytic behavior above the critical point in a random Ising ferromagnet, *Physical Review Letters*, 23 (1969), 17. [2] D. Inosov et al., Possible realization of an antiferromagnetic Griffiths phase in $\text{Ba}(\text{Fe}_{1-x}\text{Mn}_x)_2\text{As}_2$, *Physical Review B*, 87 (2013) 224425.

5:15 PM

(EMA-S7-008-2020) Thermodynamic Stability and Kinetics of Nb_3Ge , Nb_3Al , and Nb_3Ga A15 Phases

A. C. Hire^{*1}; B. Rijal¹; H. Bayard¹; C. Orozco¹; L. Zhu¹; R. Porter²; Z. Sun²; M. Liepe²; M. Manuel¹; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA
2. Cornell University, Department of Physics, USA

In this work, we investigate the thermodynamic stability and superconducting properties of Nb-based A15 phases, Nb_3Ge , Nb_3Ga and Nb_3Al . These Nb-based A15 phases can be used as potential alternatives to Nb_3Sn coatings in superconducting radio-frequency particle accelerator cavities. These A15 phases, like Nb_3Sn coatings, might lead to shorter cavity lengths, higher operating temperatures, and lower power consumption. We use a density functional theory (DFT) and cluster expansion based approach to calculate the thermodynamic stability ranges of these A15 phases. We consider two different functionals, PBE and SCAN, for the construction of the DFT based cluster expansion models and analyze their effects on the thermodynamic stability of these phases. We also perform diffusion

couple experiments to validate the stability range and determine the interdiffusion coefficients. The interdiffusion coefficient is an essential parameter in the synthesis of these A15 phases using solid-vapor or solid-liquid methods. Our calculated composition stability ranges agree with some of the experimentally determined phase diagrams. A smaller stability range is obtained in the diffusion couple experiments.

5:30 PM

(EMA-S7-009-2020) Methodological DFT Study of Spin-Crossover in $\text{Mn}(\text{taa})$

E. C. Fonseca^{*1}; D. Rodriguez²; S. Trickey²; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA
2. University of Florida, Physics, USA

Single molecular magnets present a promising materials family for quantum computing. These molecules and compounds exhibit magnetic bistability, as they can exist in two different stable spin states, making them also candidates for magnetic memory and sensors. We study the $\text{MnIII}(\text{taa})$ molecule using density-functional theory to validate the parameters of the computational methods for the spin-crossover energy and the ligand field splitting. We employ the PBE generalized gradient approximation (GGA) and SCAN meta-GGA functionals and include van der Waals corrections and the Hubbard U correction for correlation effects. We find that the choice of exchange-correlation functional drastically changes the spin crossover energy. By utilizing linear response theory, we determine the onsite Hubbard U value of the Mn-III ion for PBE+U and SCAN+U calculations. Changing the Hubbard U parameters elongates the bonds in $\text{Mn}(\text{taa})$ enough to favor a high-spin ground state. As the Mn-N bonds elongate, the ligand field splitting weakens and thus the system favors a degenerate d-orbital configuration. Due to the observed sensitivity to the choice of U value, we employ more sophisticated methods to determine the Hubbard U parameter self-consistently. Preliminary results indicate that both the PBE and SCAN functional require a Hubbard U correction to accurately predict the spin states of the $\text{MnIII}(\text{taa})$ molecular magnet.

S8: Structure-Property Relationships in Relaxor Ceramics

Perovskite/Non-perovskite Relaxors II

Room: Cypress B

Session Chair: Igor Levin, NIST

10:00 AM

(EMA-S8-014-2020) Enhanced Electromechanical Properties in Grain-Oriented Relaxor- PbTiO_3 based Piezoceramics Prepared by Templated Grain Growth (Invited)

Y. Chang^{*1}; J. Wu¹; Y. Sun¹; S. Zhang²; B. Yang¹

1. Harbin Institute of Technology, China
2. Nanjing University, China

Relaxor- PbTiO_3 based perovskites have attracted much attention over the past decades for their potential applications in ultrasonic transducers, actuators, and sensors, etc. However, relaxor- PbTiO_3 piezoceramics possess much lower electromechanical properties in comparison to the single crystals, being due to directional averaging of properties associated with randomly oriented grains. In this work, $[001]_c$ oriented relaxor- PbTiO_3 ternary ceramics with texture fraction $>90\%$ were successfully fabricated by templated grain growth. The structural variation, densification behavior, texture evolution, microstructure development, and oriented crystalline interface evolution of the templated samples during different texturing stages were investigated. The relationships among the crystallographic nature, domain structure and piezoelectricity were clarified. In contrast to the randomly oriented counterpart, significantly

enhanced electromechanical properties ($d_{33}^* = 1555$ pC/N, $d_{33} = 824$ pC/N, and $k_p = 0.81$) and high ferroelectric properties ($E_c = 8.3$ kV/cm and $P_r = 31$ μ C/cm²) were obtained from those highly textured ceramics. We believe that this work can largely broaden device application areas of relaxor-PT based ceramics.

10:30 AM

(EMA-S8-015-2020) Enhancing the electromechanical response of relaxor films through aerosol deposition of metal electrodes (Invited)

N. Khansur¹; U. Eckstein¹; H. Uršič²; K. G. Webber^{*1}

1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Science and Engineering, Germany
2. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia

(Na_{1/2}Bi_{1/2})TiO₃-based lead-free ferroelectrics show promise for actuation systems due to a large unipolar strain, but are limited by their poling field and low depolarization temperature. A number of strategies have been proposed, which have increased the electromechanical response but also resulted in some additional limitations, e.g., reduction in depolarization temperature or increased porosity. In this presentation, a new method will be introduced for increasing the unipolar strain and depolarization temperature as well as reducing of poling field of polycrystalline (Na_{1/2}Bi_{1/2})TiO₃-0.07BaTiO₃. Room temperature aerosol deposition (AD) was used to deposit copper electrodes, resulting in the formation of residual stress that induced long-range ferroelectric order. These stresses increased the electromechanical properties as well as the thermal stability, which will be shown through macroscopic strain-electric field and temperature-dependent dielectric measurements. The stress-modulated relaxor-ferroelectric transition will be discussed in conjunction with the development of internal residual stresses in functional ceramics during AD. Piezoresponse force microscopy will be used to show the evolution of ferroelectric domains in NBT-7BT following AD, which will be compared to ex situ stress-dependent PFM to provide insight into the stress distribution through the thickness.

Novel Relaxors

Room: Cypress B

Session Chairs: Igor Levin, NIST; Mael Guennou, University of Luxembourg

11:00 AM

(EMA-S8-016-2020) High Energy Density Capacitors (Invited)

I. M. Reaney^{*1}

1. University of Sheffield, Materials Science and Engineering, United Kingdom

Ultrahigh discharge energy density ($W_{dis} = 10.5$ J/cm³) and efficiency ($\mu = 87\%$) have been obtained in doped BiFeO₃-BaTiO₃ ceramic multilayers by achieving an electrically rather than chemically homogeneous microstructure. Back scattered scanning and transmission electron microscopy combined with energy dispersive X-ray spectroscopy mapping of (0.7-x)BiFeO₃-0.3BaTiO₃-xNd(Zn_{0.5}Zr_{0.5})O₃ (0.05 < x < 0.10) ceramics revealed a core-shell grain structure which switched from a bright to dark contrast as x increased. Compositions with x = 0.08 were at the point of cross over between these two manifestations of core-shell contrast. Dielectric measurements together with the absence of macrodomains in diffraction contrast TEM images suggested that compositions with x = 0.08 exhibited relaxor behaviour within both the core and shell regions. Impedance spectroscopy demonstrated that, despite being chemical dissimilar, the grains were electrically homogeneous and insulating with little evidence of conductive cores. Multilayers of x = 0.08 had enhanced breakdown strength, $E_{BDS} \sim 700$ kV/cm and a slim hysteresis loop which resulted in large W_{dis} and high μ , temperature stable to 15% from 25 to 150 °C.

11:30 AM

(EMA-S8-017-2020) Electric field induced strain in Sr(Hf_{0.5}Zr_{0.5})O₃-modified Bi_{0.5}(Na_{0.8}K_{0.2})_{0.5}TiO₃ piezoelectric ceramics

S. K. Gupta^{*1}; R. McQuade¹; B. Gibbons¹; P. Mardilovich²; D. Cann¹

1. Oregon State University, Material Science, School of Mechanical, Industrial, and Manufacturing Engineering, USA
2. Xaar plc, United Kingdom

Lead-free Sr(Hf,Zr)O₃-modified Bi_{0.5}(Na_{0.8}K_{0.2})_{0.5}TiO₃ ceramics were synthesized using conventional solid-state mixed-oxide method. The XRD data revealed a pure perovskite phase throughout the studied compositional range. Coexistence of tetragonal and rhombohedral phases was observed for x=0 and, with the addition of SHZ, a phase transition to a pseudocubic phase was observed. Ferroelectric, dielectric and electric-field-induced strain behavior was also studied as a function of composition. The temperature dependent-dielectric spectra showed frequency dependence for all the SHZ-modified BNKT ceramics which is a typical characteristic of relaxor ferroelectric. Furthermore, constriction in polarization loops and an absence of negative strain in the bipolar strain measurement for SHZ-modified BNKT compositions indicate that the addition of SHZ significantly disrupts the ferroelectric order. In particular, the addition of 2 mol% SHZ in BNKT markedly enhanced the electric-field-induced strain from 0.10% (for pure BNKT) to 0.33%. The corresponding normalized strain coefficient ($d_{33}^* = S_{max} / E_{max}$) increased from 196 pm/V to 663 pm/V at a moderate electric-field of 50 kV/cm. These results indicate that BNKT-SHZ ceramics can be designed for an improved strain response via a substitution-induced relaxor state for high performance, lead-free electromechanical actuator applications.

Advanced Characterization of Relaxors

Room: Cypress B

Session Chairs: Igor Levin, NIST; Mael Guennou, University of Luxembourg

11:45 AM

(EMA-S8-018-2020) Large electromechanical response in non-MPB relaxor ferroelectrics

R. Ranjan^{*1}; U. Shankar¹; R. Pandey¹; B. Narayan¹

1. Indian Institute of Science, Materials Engineering, India

Large electromechanical response in ferroelectric solid solutions is generally associated with a composition driven inter-ferroelectric instability, commonly known as morphotropic phase boundary (MPB). In contrast to this general perception, we show that large electromechanical response is possible even in non-MPB relaxor ferroelectric systems. We demonstrate this on three ferroelectric solid solution systems namely (1-x)PbTiO₃-(x)Bi(Ni_{1/2}Hf_{1/2})O₃ (PT-BNH), (1-x)PbTiO₃-(x)Bi(Ni_{1/2}Zr_{1/2})O₃ (PT-BNZ) and (Bi,Li)FeO₃-PbTiO₃ (BF-PT:La). While the first two systems PT-BNH and PT-BNZ show $d_{33} \sim 400$ -450 pC/N, BF-PT:La shows an extraordinarily high electrostrain of $\sim 1.3\%$ in the polycrystalline ceramic form. While analogous to the conventional MPB systems, the critical compositions of these alloys mimic a two-phase structural state (cubic + tetragonal) on the global scale, detailed analysis suggests that it is not so. The cubic phase is rather a manifestation of short correlation length of the tetragonal regions and appears when the system is compositionally driven from a normal ferroelectric state to a relaxor ferroelectric state. In the absence of MPB, the polarization rotation is not likely to be the important mechanism contributing to large electromechanical response of these systems. We argue that the large response is associated with domain wall motion, large local polarization, and a (non-MPB) lattice softening.

12:00 PM

(EMA-S8-019-2020) Multiscale characterization of lead-based relaxor ferroelectrics (Invited)M. Otonicar^{*1}; A. Bradesko¹; M. J. Cabral³; L. Riemer⁴; H. Uršič¹; A. Bencan¹; G. Drazic²; J. L. Jones³; D. Damjanovic⁴; B. Malic¹; T. Rojac¹

1. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia
2. National Institute of Chemistry, Slovenia
3. North Carolina State University, Dept. of Materials Science & Engineering, USA
4. Swiss Federal Institute of Technology in Lausanne - EPFL, Ceramics Laboratory, Switzerland

The best known and widely investigated relaxor ferroelectrics are lead-based perovskites. Typically, Pb^{2+} is present on the A-site of the ABO_3 perovskite structure and mixed occupancy of cations of different size and charge is found on B-site (e.g., $(Pb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3)$, PMN-PT). In the tetragonal PMN-PT compositions ($x > 0.35$) Ti^{4+} is believed to increase charge ordering, leading to long-range ferroelectric order, while the monoclinic (M) compositions (up to $x \sim 0.35$ PT) seem to be strongly affected by both B-site disorder as well as local off-centring of Pb^{2+} . In this contribution I will show differences between the two compositional regions of PMN-PT, which are effectively observed on the local scale by atomic resolution microscopy. Moreover, microscopic observations show characteristic domain structures with hierarchically arranged nanodomains on the M side, with highly mobile nanodomains when the electric field is applied. Consistent with this finding, macroscopic measurements of the weak-field-induced polarization and strain response show distinct features in the M compositions, i.e., a strongly nonlinear and hysteretic response, which is confined to the compositions where the dielectric response shows relaxor-type frequency dispersion. All these multiscale measurements indicate the influence of local charge disorder on the mesoscale structure, as well as on the global behaviour of relaxor ferroelectrics.

S9: Ion Conducting Ceramics**Ion Conducting Ceramics for Solid-State Battery**

Room: Citrus A

Session Chairs: Hua Zhou, Argonne National Lab; Yingge Du, PNNL

2:00 PM

(EMA-S9-001-2020) Li dendrite suppression in solid state electrolytes (Invited)C. Wang^{*1}

1. University of Maryland, Chemical Engineering, USA

Solid electrolytes (SEs) are believed to prevent Li dendrite growth because of high mechanical strength and high Li^+ transference number. However, the growth of lithium dendrites is facilitated in LLZOs and LPSs as evidenced by a low critical current densities. The mechanism for lithium dendrite formation and growth in LLZO and LPS is still disputable. The lack of understanding the Li dendrite formation mechanism seriously impeded the development of solid-state lithium batteries. We demonstrated that the Li dendrites can either grow into solid electrolytes from Li anodes or directly deposit inside of solid electrolyte depending on the electronic conductivity, interface energy of solid electrolyte to Li, and electrolyte modulus. To suppress Li dendrite growth in the solid electrolytes, the electrolytes should have a high interface energy or form a SEI with high interface energy against Li with a low electronic conductivity. By introducing an electronically insulating LiF SEI between Li and LPS, we effectively suppressed Li dendrite growth in the LPS electrolytes because the LiF is thermodynamically stable with Li and has a high interfacial energy with Li. In addition, the extremely low electronic conductivity of LiF can also inhibit the Li plating inside LPS by blocking the electronic conduction pathway.

*Denotes Presenter

2:30 PM

(EMA-S9-002-2020) Structure, Chemistry, and Charge Transfer Resistance of the Interface between Garnet Solid Electrolyte and Oxide Cathodes (Invited)B. Yildiz^{*1}

1. Massachusetts Institute of Technology, USA

All-solid-state batteries promise significant safety and energy density advantages over liquid-electrolyte batteries. The interface between the cathode and the solid electrolyte is an important contributor to charge transfer resistance. Strong bonding of solid oxide electrolytes and cathodes requires sintering at elevated temperatures. Knowledge of the temperature dependence of the composition and charge transfer properties of this interface is important for determining the ideal sintering conditions. To understand the interfacial decomposition processes and their onset temperatures, model cathode systems of $LiCoO_2$ (LCO) and $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622) thin films deposited on cubic Al-doped $Li_7La_3Zr_2O_{12}$ (LLZO) pellets were studied as a function of temperature, gas composition and electrochemical conditions. The methods combine interface-sensitive techniques, including X-ray photoelectron spectroscopy (XPS), synchrotron X-ray absorption spectroscopy, hard X-ray photoemission (HAXPES), and synchrotron X-ray diffraction. In this talk, we will present the found precipitation products at the interface as a function of synthesis and electrochemical conditions, their role in altering the interface resistance to Li transfer, and compare the LCO and NMC related cathodes in terms of their instability onset conditions.

3:00 PM

(EMA-S9-003-2020) Synthetic Designs for Improved NaSICON Sodium Ion ConductorsE. Spoerke^{*1}; A. Peretti¹; E. Coker¹; M. Rodriguez¹; M. Gross¹; J. A. Bock¹; R. Hill²; Y. Cheng²

1. Sandia National Laboratories, USA
2. University of Kentucky, USA

Robust, high conductivity, solid state separators are key elements of emerging solid-state and molten metal batteries. Here, we discuss insights into the synthesis and properties of the solid-state sodium ion conductor, NaSICON (nominally, $Na_3Zr_2PSi_2O_{12}$), a promising ceramic separator, particularly for lower temperature applications ($< 200^\circ C$). Effective NaSICON performance is strongly dependent on its phase purity and sintered density, which are difficult to control during synthesis. We employ thermal analyses, such as variable temperature x-ray diffraction, thermogravimetric analysis, and differential thermal analysis, to inform the controlled reactive sintering of NaSICON. We then evaluate how variations in ceramic processing and composition affect key properties such as ionic conductivity, density, and mechanical behavior. Optimized materials are subsequently utilized in prototype molten sodium batteries, where these properties translate to functional performance. This rationally-designed synthesis will be central to producing highly functional NaSICON separators for safe, reliable new battery technologies. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

3:15 PM

(EMA-S9-004-2020) Interfacial Engineering of Ceramic Separators in Sodium BatteriesM. Gross^{*1}; A. Peretti¹; S. Percival¹; L. Small¹; E. Spoerke¹

1. Sandia National Laboratories, USA

High sodium-ion conductivity ceramic separators are a key component to the development of low temperature ($< 150^\circ C$) molten sodium batteries. Conventional Na^+ -ion conducting separators

such as β - Al_2O_3 or NaSICON typically require high operating temperatures, not only for improved ionic conductivity, but also to allow greater wetting of the molten sodium anode to the ceramic. Lowering the temperature from ~ 300 °C to near 100 °C leads to poor interfacial wetting of molten sodium to the ceramic separator, which results in high cell resistance and poor battery performance. Here, we describe our efforts to modify the interface between the molten sodium and the Na^+ -ion conducting separator for improved wetting in batteries cycling at low operating temperatures. We explore the use of engineered coatings on the ion-conducting ceramic to improve molten sodium wetting and to dramatically reduce cell-limiting interfacial resistance. This strategy offers great promise towards enabling operation of molten sodium batteries at low temperatures. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

4:00 PM

(EMA-S9-013-2020) Fast Charging Ceramic Anodes for Aqueous Sodium-Ion Batteries (Invited)

Z. Feng^{*1}

1. Oregon State University, School of Chemical, Biological, and Environmental Engineering, USA

Aqueous sodium-ion batteries are attractive battery alternatives for stationary energy storage due to their inherently low cost and high safety. The development of advanced electrode materials with excellent performance and low cost is crucial for the success of aqueous Na-ion batteries. Our group has recently studied several types of iron phosphate based ceramic electrodes as promising anodes alternative for aqueous Na-ion batteries. We found these anodes can exhibit very fast ionic diffusion that enables the fast charging rate, long cycle life, high capacity retention and rate capability. In combination of electrochemical characterization and multimodal synchrotron X-ray scattering and spectroscopy methods, we further reveal the reaction mechanism associated with these high performance ionic conducting ceramics. Our work also underlines the importance of fabricating aqueous batteries on the basis of the Earth-abundant, cost-effective, and non-toxic elements.

4:30 PM

(EMA-S9-006-2020) Microstructural evolution and fracture strength of sintered $\text{Li}_4\text{Ti}_5\text{O}_{12}$ -Ni anode composites

W. Huddleston^{*1}; F. Dynys²; A. Sehirlioglu³

1. Case Western Reserve University, Department of Materials Science and Engineering, USA
2. NASA Glenn Research Center, USA
3. Case Western Reserve University, USA

Next generation aerospace concepts leverage multifunctionality to achieve systems-level weight savings. Co-processing of strain-free $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode and nickel metal current collector was investigated for application in a load bearing structural battery. High bulk density and percolation of current collector were sought to achieve structural integrity and high electrical conductivity. Evolution of nickel current collector particle size distributions during sintering of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ -Ni anode composites was analyzed as a function of processing conditions and composite composition. Application of Ostwald ripening theories to average particle size coarsening provided microstructural modeling and identification of transport mechanisms, while incorporation of particle interaction effects was achieved by fitting of particle size distributions. A measured activation energy of 1.06 eV was correlated with boundary transport of nickel. Complex fitting observed the formation of bimodal particle size distributions in compositions above the percolation threshold

and for samples sintered at high temperatures and with long dwell times, indicating interactions between neighboring particles during sintering. Mechanical fracture strength was measured by ring-on-ring testing as a function of nickel content, bulk density, and particle size.

4:45 PM

(EMA-S9-007-2020) Controlled Processing-Structure-Properties of Two-Dimensional Oxides

K. Pachuta^{*1}; E. Pentzer²; M. Berger³; A. Sehirlioglu⁴

1. Case Western Reserve University, Materials Science and Engineering, USA
2. Texas A&M University, Materials Science and Engineering, USA
3. MINES ParisTech, Mécanique et Matériaux, France
4. Case Western Reserve University, USA

Two-dimensional (2D) materials have gained steady interest in the materials science community since the discovery that many layered materials, such as graphite, layered chalcogenides, and layered oxides can be readily stabilized into their 2D state. Owing to their exciting properties when compared to the bulk, 2D materials show promise in many applications in electronic devices, sensors, energy generation and storage, etc. With many novel 2D materials being produced today – and not all of them are coming from layered precursors – the field is growing at an astonishing rate, yet still only a few 2D materials (graphene, hexagonal-boron nitride, manganese oxide, etc.) have been extensively studied for their structure and related properties. Additionally, certain exfoliation/synthesis/deposition methods can alter the inherent structure, defects, and related properties of a 2D material. In this work, the exfoliation of layered oxides is examined relating how the exfoliation methods presented may compare to relevant synthesis and deposition techniques to produce the same material. Using the exfoliation of lithium cobalt as its primary example, this work demonstrates how observations made using characterization techniques such as UV-Vis spectroscopy, Transmission Electron Microscopy, Scanning Electron Microscopy, X-ray Diffraction, etc. may help decipher the processing-structure-property landscape of 2D oxides.

5:00 PM

(EMA-S9-008-2020) Improving the Lithium-Ion Battery Performance through Surface Coating

M. Lucero^{*1}; T. Holston¹; Z. Feng²

1. Oregon State University, Chemical Engineering, USA
2. Oregon State University, School of Chemical, Biological, and Environmental Engineering, USA

Lithium-ion batteries (LIBs) are the most popular rechargeable batteries in portable electronics and have made their way into the electric vehicle and grid storage market. Despite wide applications of LIBs, there is still room for improvement in terms of capacity retention and energy density. We utilize a sol-gel synthesis to successively deposit two surface coating layers ($\text{Li}_2\text{SrSiO}_4$ & Al_2O_3) on LiCoO_2 cathode. We demonstrate that the dual coating can improve the electrochemical performance at a higher cut-off potential of 4.5 V, e.g. larger capacity (190 mAh/g), and better capacity retention of (64% after 500 cycles) at 0.5C using commercial electrolyte (LiPF_6). The cathode-protected LIB also exhibits excellent rate capacity (up to 10 C). In addition, the role of the dual coating is investigated by a combination of electrochemical, surface-sensitive spectroscopy, and microscopy characterization techniques.

S10: Point Defects and Transport in Ceramics

Defect Mediated Properties (Conductivity, Grain Growth, Creep, Magnetism, Ferroelectric Imprint, Dielectric Degradation)

Room: Citrus A

Session Chair: Douglas Irving, North Carolina State University

10:00 AM

(EMA-S10-016-2020) Affecting point defects in SrTiO₃ by illumination and preparation (Invited)

J. Fleig*¹

1. TU Wien, Chemistry, Austria

The defect chemical understanding of SrTiO₃ is rather advanced, particularly for the equilibrated bulk of slightly doped samples. However, defect concentrations may deviate from the expected bulk values due to several reasons, even if equilibrium with the gas phase is established: First, close to interfaces, space charges come into play. Second, cation defects are often frozen-in and their concentration in the actual measurements depends on the sample prehistory (sintering temperature and preparation procedure, particularly for thin films prepared by PLD). Third, illumination affects the electronic charge carrier concentrations and thus also modifies ionic defect concentrations in (quasi-)equilibrium with the gas. In this contribution, novel results on such less common or unexpected defect related phenomena in SrTiO₃ are presented: i) The relevance of Sr vacancies in undoped SrTiO₃ bulk samples is considered and defects in space charges are compared for undoped and Fe-doped single crystals. ii) Unusually low conductivities in doped SrTiO₃ thin films are examined and the role of cation non-stoichiometry in such films is discussed. iii) The effect of UV light on the defect chemical properties is presented; here several different phenomena are compared: conductivity changes, color changes, voltage changes in electrochemical cells with SrTiO₃ electrodes and voltage changes in solar cells based on SrTiO₃.

10:30 AM

(EMA-S10-017-2020) Engineering defect formation in functional oxide thin films and heterostructures (Invited)

R. Dittmann*¹

1. Forschungszentrum Juelich, PGI-7, Germany

The precise control over the defect configuration is one of the key challenges for oxide-based electronic thin film devices. Defect formation during pulsed laser deposition growth can be either governed by the defect equilibria at the given growth conditions or by the plume dynamics, the presence of UV-irradiation [1] or by the growth kinetics. We will present detailed studies on selected prototypical oxide thin film systems which enabled us to disentangle the different factors influencing the formation of both, oxygen and cation vacancies. We observe a significant influence of the surface termination of SrTiO₃ single crystal substrates on the formation of oxygen vacancies during annealing and growth and attribute it to the inhibited surface exchange for SrO-terminated SrTiO₃ [2]. By investigating the early stage of growth by in situ AFM and RHEED we could reveal the complex interplay between non-stoichiometry, growth mode and the formation of extended defects such as antiphase boundaries and Ruddlesden-Popper-type of defects [3]. We will furthermore give examples how defect engineering can be employed to fabricate thin film devices with tailored functional properties [4].

11:00 AM

(EMA-S10-018-2020) Defect Chemistry of Na_{0.5}Bi_{0.5}TiO₃-based ceramics: Changing ferroelectric properties and inducing high ionic conductivity (Invited)

S. Steiner¹; L. Koch¹; A. Hoang¹; M. Gehringer¹; K. Albe¹; T. Frömling*¹

1. Technische Universität Darmstadt, Materials Science, Germany

Ceramics based on Na_{0.5}Bi_{0.5}TiO₃ (NBT) have been shown to be excellent lead-free ferroelectrics and relaxor materials. The defect chemistry of NBT-ceramics is, however, quite complex. They can actually be tuned from highly ionically conductive to highly resistive. For example, acceptor doping does not lead to the hardening of ferroelectric properties as it was initially expected. Instead, mobile oxygen vacancies are induced making the material an excellent oxygen ion conductor. Even though this is quite interesting from a research perspective it can be very detrimental for the transfer of NBT-ferroelectrics into application. Aging and fatigue models from other well-known ferroelectrics might not be applicable. Thus, a detailed understanding of the defect chemistry of NBT and its solid solutions is of great importance. In this work, a model to rationalize the defect chemistry of NBT-ceramics will be presented. Furthermore, methods to control the ionic conductivity, ferroelectric properties and the microstructure will be discussed. It will be shown that even excellent high temperature capacitor material having highest requirements considering dielectric loss can be derived from NBT. This will illustrate the extraordinary opportunities to alter properties of NBT-based material for multiple applications.

11:30 AM

(EMA-S10-019-2020) Reversibility of Electromagnetic properties in La_{0.8}Sr_{0.2}MnO₃ Thin Films from High Temperature Processing

D. Lau*¹; J. Wuenschell¹; J. Devkota¹; P. Ohodnicki¹

1. National Energy Technology Laboratory, USA

Complex perovskite oxides such as La_{0.8}Sr_{0.2}MnO₃ (LSMO), have attracted interest for emerging optical, electronic, and magnetic device applications due to their unique electromagnetic properties which are directly tied to their electronic band structure. Recent work has combined the high temperature stability with unique optical and electronic properties for applications in monitoring of gas stream chemistry (i.e. oxygen concentration) internal to a high temperature process environment. In this work, we illustrate the relationship between the functional properties in LSMO thin films as a function of crystallographic texture and high temperature in various gas atmospheres. Specifically, we systematically characterize LSMO thin films grown on SrTiO₃, LaAlO₃, (LaAlO₃)_{0.3}(Sr₂AlTaO₆)_{0.7}, and MgO substrates using RF magnetron sputtering and report on transport properties in the DC and AC regimes as well as magnetic properties. Measurements are performed using magnetometry, four-point probe, and electrical impedance spectroscopy at ambient conditions as well as in-situ gas environments of varying oxygen concentration at elevated temperatures. Reversible cycling in electrical transport and magnetic properties are observed and attributed to compositional and structural changes in LSMO as oxygen vacancies are generated or removed in high temperature gas environments.

11:45 AM

(EMA-S10-020-2020) Defect Kinetics in (Bi_{0.5}Na_{0.5})TiO₃-based piezoceramics

Z. Fan*¹

1. Pennsylvania State University, USA

Point defects, to a certain extent, determine the performance of piezoelectric ceramics. Owing to the volatility of Bi and Na, (Bi_{0.5}Na_{0.5})TiO₃ (BNT) is naturally complicated in terms of the defect chemistry. Of particular interest is the sensitivity to the processing condition. Upon cooling in air, superoxidation occurs

at low temperature and low cooling rate, of which the state can be controlled via quenching from different annealing conditions. The superoxidation-dependence of mixed electronic-ionic conduction is analyzed with impedance spectroscopy. On top of the electrical insulation, polarization fatigue is also a defect-related issue. The fatigue resistance in BNT has been found significantly affected by the phase-composition. In-situ transmission electron microscopy (TEM) is employed to compare the fatigue behaviors in two BNT-based samples which are ergodic and nonergodic relaxor phase, respectively.

12:00 PM

(EMA-S10-021-2020) Engineering defects for electro-active applications (Invited)

P. Janolin^{*1}; Z. Li¹; J. Yu¹

1. CentraleSupélec-CNRS, Physics, France

Point defects such as oxygen vacancies are usually detrimental to functional insulators with applications based on electro-strains or used to store energy. Nevertheless they can be beneficial in some specific contexts and their benefit can be harnessed through defect engineering, exploiting the symmetry-comforming principle. In this presentation, two examples shall be given: - the first one deals with the control of the polarisation vs electric field loop in ferroelectrics through aliovalent doping, thereby introducing oxygen vacancies. The ability to shift the hysteresis cycle through defect engineering represents a promising avenue to obtain self-polarised ferroelectrics or increase their energy storage capacity. - the second one is about the “giant” electrostriction phenomenon. Materials having electrostrictive coefficients (relating the electric-field-induced deformation to the square of the dielectric displacement) several orders of magnitude larger than what would be expected from the universal empirical law have recently been discovered. The basic mechanism remains to be unravelled by the role of oxygen vacancies, distorting heavily the host lattice, though at the local scale, and their response to an applied electric field, appears at the hear of this exacerbated response.

S12: Electronic Materials Applications in 5G Telecommunications

5G Measurement Science

Room: Cypress C

Session Chair: Geoff Brenneka, Colorado School of Mines

10:00 AM

(EMA-S12-017-2020) VNA replacements to be used in measurements of material properties performed in the mm-wave and sub-THz bands (Invited)

P. Kopyt^{*1}; B. Salski²

1. Warsaw University of Technology, Inst. of Radioelectronics and Multimedia Technology, Poland
2. Warsaw University of Technology, Poland

The paper describes measurement setups allowing one to measure over the Ka-band and parts of the WR-10 band the scalar transmission coefficient of a state-of-the-art high-Q Fabry-Pérot open resonators that are often used for measurement of properties of low-loss materials. Both setups described herein employ readily-available components. Their performance is verified against measurements performed using a laboratory-grade vector network analyzer for two exemplary material samples and agreement is found, which demonstrates that an effective material properties measurement system can be realized also without high-end laboratory equipment which open ways for available characterization of samples in cost-sensitive applications.

10:30 AM

(EMA-S12-018-2020) Broadband dielectric characterization of polymers and ceramics (Invited)

M. Lanagan^{*1}; M. Sarkarat²; T. Bonnett¹; S. Shetty²; B. Foley²; S. Perini²

1. Pennsylvania State University, Dept. of Engineering Science and Mechanics, USA
2. Materials Research Institute, USA

We have explored dielectric measurement methods spanning the frequency range between 1 MHz and 100 GHz. Two general types of measurement techniques, resonant and transmission, have been developed. Resonant methods are generally discrete frequency measurements that have high accuracy, specifically for low loss dielectrics with dissipation factors below 1%. We have established several resonant methods: a dielectric post technique in the 1-10 GHz range, a split-cavity method between 15-20 GHz and a Fabry-Perot method between 20-40 GHz. Transmission/reflection methods have the advantage of being broadband and cover a large frequency range (1MHz to 110 GHz). However, the dielectric loss accuracy limits transmission line methods to high loss samples. We have developed a reflection method for the 1 MHz to 2 GHz frequency range, where polymers and polymer composites display significant dielectric relaxation. Furthermore, quasi-optical measurement of these materials from 75 – 110 GHz is performed and compared with the various methods, motivated by eventual applications within this frequency range.

11:00 AM

(EMA-S12-019-2020) Hexaferrite Thin Film Growth on Sapphire and Semiconductor Substrates for mm-wave Applications

P. Kulik^{*1}; C. Yu¹; A. Sokolov¹; G. Winter¹; V. Harris¹

1. Northeastern University, ECE, USA

The demand for miniaturized and high performing broadband communication systems in the GHz frequency range is steadily growing due to severely crowded and rapidly changing modern commercial and defense spectral environments. In this work, we demonstrate for the first time a complex Z-type hexaferrite film grown on various substrates including sapphire using pulsed laser deposition (PLD). A thin-film Z-type hexaferrite can result in low microwave loss and high hysteresis loop squareness required for the design of self-biased RF devices such as circulators in which external permanent magnets are removed from the circuit. The polycrystalline Co₂Z ferrite target, having a nominal composition of Ba₃Co₂Fe₂₄O₄₁ was prepared by a solid state process. Then, pulsed laser deposition was performed for one hour to deposit 1 micron of film on a sapphire substrate. XRD characterization confirms that the thin film is a pure-phase Z-type and matches that of the target. Further process refinement such as annealing shows improvement in hysteresis loop squareness. Material integration for device will be studied in further detail.

11:15 AM

(EMA-S12-020-2020) Characterization of dielectric materials for 5G telecommunications with a Fabry-Perot open resonator (Invited)

B. Salski^{*1}; T. Karpisz¹; P. Kopyt¹; J. Krupka²

1. Warsaw University of Technology, Institute of Radioelectronics and Multimedia Technology, Poland
2. Warsaw University of Technology, Institute of Microelectronics and Optoelectronics, Poland

It is shown in this paper that a Fabry-Perot open resonator can be applicable to broadband characterization of low-loss dielectric materials exploited in 5G telecommunications. Although the concept of the method had been known for years, only recently a novel approach to the measurement procedure been proposed, which allows reducing measurement inaccuracy at no cost of increased computational effort. For that purpose, a new scalar

one-dimensional electromagnetic model of the resonator has been proposed, the results of which are compared with measured data to evaluate, in turn, the unknown complex permittivity of a sample. Another challenge that has been solved is robust mode identification and tracking, which is essential due to the fact that the resonator is electrically long, so there are plenty of spurious modes. The whole measurement process is fully automated so that the only needed user intervention is insertion of the sample, which should be in the form of a laminate with the diameter of over 3 inches. The operation of the system is shown by measuring materials well-known in 5 G applications, such as silicon or fused silica.

11:45 AM

(EMA-S12-021-2020) Free-Space Material Measurements at 20-40 GHz: RF Spot Probes vs. a Lens-Based Focused Beam System

J. W. Schultz^{*1}; J. G. Maloney²; A. A. Patel¹

1. Compass Technology Group, USA
2. Maloney-Solutions, USA

A method for microwave and millimeterwave characterization of materials is the free-space focused beam technique, which uses lenses or shaped reflectors to focus energy onto a confined region of a material specimen. In these fixtures, lenses form a Gaussian focused beam with plane-wave like characteristics at the focal point. This method has proved popular because of its wide bandwidth and flexibility. Another free-space measurement technique employed by some is the use of dielectrically loaded antennas placed in close proximity to a specimen. In this alternate technique, the dielectrically loaded antennas are smaller than lenses, making the hardware more compact and lower cost, however this is done at the expense of some reduced accuracy. This paper compares a standard laboratory focused beam system to some recently developed millimeterwave spot probes. The spot probes are specially designed antennas encapsulated in a solid dielectric and optimized to provide a small illumination spot three to eight centimeters in front of the probe. Experimental measurements of several dielectric and resistive specimens were measured by both systems for direct comparison. Additionally, comparisons were made with both fixtures to establish measurement limits and capability differences between the two methods.

12:00 PM

(EMA-S12-022-2020) Resonant Cavity Measurement for use in a Free Space System for the Characterization of Low Loss Materials (Invited)

C. Kintner¹; C. Garcia¹; A. Updegrave^{*1}

1. Ball Aerospace, USA

It is well known that nonuniform fields significantly affect the ability to characterize dielectrics by microwave cavity perturbation. Orloff et. al. showed that the microwave cavity perturbation method can be greatly improved by fitting data of various filling fractions. It was shown that this can increase the characterization by an order of magnitude. Ball Aerospace and NIST have partnered to integrate free space measurements and the above method. By combing these methods, we will show improved characterization of low loss materials which will enable improved electromagnetic design in an industry setting. The resonant cavity design was simulated in a full wave electromagnetic solver, prior to fabrication and its performance was validated. To verify this novel method, well understood ceramic and organic materials in high frequency design were selected to be characterized.

12:15 PM

(EMA-S12-023-2020) Microwave-frequency material dielectric properties measurements at elevated temperature (Invited)

C. Ellison^{*1}; R. Tempke²; M. Spencer¹; C. Wildfire¹; T. Musho²; D. Shekhawat³

1. National Energy Technology Laboratory / Leidos Research Support Team, USA
2. National Energy Technology Laboratory / Oak Ridge Institute for Science and Education, USA
3. National Energy Technology Laboratory, USA

Dielectric properties of materials are important across many sectors and applications in the understanding of the fundamental interactions between electromagnetic radiation and materials. At NETL, dielectric characterization of catalyst materials assists in basic understanding of microwave phenomena that result in rate enhancement, shifted product conversions, and improved efficiencies, which are not observed under conventional thermal heating. In addition, dielectric material properties are input into numerical simulations used to model microwave systems. As material dielectric properties are temperature dependent, it is important to characterize the dielectric properties at the material's operating temperature to obtain accurate permittivity values. Measurement at high temperature is challenging because most measurement equipment can be damaged by higher temperatures, so it is necessary to isolate the sensitive components from the heated material. This presentation will discuss our lab group's material measurement work based on coaxial airline measurement technique from 0.1 to 13.5 GHz and our modification of this test fixture for dielectric properties measurements at high temperatures. Benefits and limitations of this setup will be discussed. Also, an overview of the microwave applications being investigated at NETL will be presented.

Industry Panel and Tutorials

Room: Cypress C

Session Chair: Geoff Brenneka, Colorado School of Mines

2:30 PM

(EMA-S12-024-2020) DC to THz Electromagnetic Properties Characterization (Invited)

S. Phommakesone^{*1}

1. Keysight Technologies, USA

From stealth materials to dielectric substrates, microwave food products to biofuels, accurate characterization of their electromagnetic properties from DC to THz frequencies provide engineers with critical information needed for material and circuit design, modeling, new material research, health and safety, manufacturing, quality control, and more. Many measurement methods exist, but which to choose is often a mystery. My intent with this paper is to clear the air by providing an overview of each measurement method, with its strengths and limitations. Typically, the measurement is made with vector network analyzer, where dielectric and magnetic properties of materials are calculated from measured S-parameter. Therefore, the whole measurement system (RF instrument, fixture, and software) and setup considerations will also be covered.

3:00 PM

(EMA-S12-025-2020) Tutorial: How to measure permittivity on-wafer

N. Orloff^{*1}

1. NIST, Communications Technology Laboratory, USA

In this talk, I will go through step-by-step how to perform on-wafer measurements and extract the permittivity of materials with on-wafer measurement science. I will start by discussing how to use the NIST calibration wafer with free NIST software. Then, I will

step through the types of devices used to extract permittivity. I will discuss our device layouts and how to measure the devices. Next, I will go through the on-wafer calibrations, materials characterization measurements, and the resulting measurands used to quantify a materials permittivity. I will go through the finite-element simulations used to obtain the permittivity as a function of frequency and finally obtain the permittivity of a well-known material. As part of this talk, I will distribute on-wafer calibration kits and how to use them.

3:15 PM

(EMA-S12-026-2020) Nanoscale Materials Characterization for Microwave and mm-Wave Applications (Invited)

T. M. Wallis^{*1}; S. Berweger¹; P. Kabos¹

1. National Institute of Standards and Technology, Applied Physics Division, USA

Innovations in material science are crucial for the ongoing development of faster, high-throughput wireless communications at microwave and mm-wave frequencies. New materials systems must be optimized across atomic, microscopic, and macroscopic length scales. In recent decades, near-field scanning microwave microscopy (NSMM) has emerged as a powerful tool for local microwave materials characterization at nanometer lengths scales. NSMM instrumentation combines broadband microwave (and mm-wave) compatibility with the spatially-resolved measurement capabilities of scanning probe microscopes. Recent advances in instrumentation have led to improved sensitivity for measurements of a variety of material parameters, including sheet resistance, complex permittivity, as well as carrier type and concentration. Here, we will use several case studies to demonstrate and review the capabilities of this technique. For example, NSMM has been used to image gate-voltage-controlled, coexisting domains of n- and p-type regions in ambipolar tellurene transistors. Further, NSMM has been used to image spatial variations in electronic properties of pristine and degraded methylammonium lead-halide perovskite films. Finally, with the aid of custom-engineered calibration structures, NSMM can extract local measurements of microwave impedance, which in turn can be used to estimate the local complex permittivity.

3:30 PM

(EMA-S12-027-2020) Exploring synergies between electronic material measurements and modeling (Invited)

M. Celuch^{*1}; M. Olszewska-Placha¹; J. Rudnicki¹

1. QWED Sp. z o.o., Poland

Electromagnetic simulators have become indispensable design tools for mm-wave communications. However, simulation results can only be as good as material data fed into the simulator, and telecommunication engineers well realize the need for accurate methods of material measurements at GHz frequencies. It is not so broadly realized that a measurement is not a revelation, but remains subject to similar constraints as a simulation. Behind each measurement, there is a model of the physical processes assumed to be taking place in the material, and the measurement serves to identify that model parameters. Hence, a reliable simulation of the measured scenario is needed to validate the constructed model under a range of conditions. Despite such bilateral links, the two worlds of material measurements and computer modelling are mostly advanced by separate groups of researchers. In this talk, we report our works within the European H2020 MMAMA project, aiming to bring the two worlds closer together. We focus on the resonant methods of dielectric measurements and present new models (e.g. industrial CAD formats translated into conformal FDTD meshes) and simulation procedures (e.g. near-field-imaging) that support their understanding (of e.g. SPDR and SiPDR techniques) and developments (e.g. downscaling of surface scans). We discuss grid-search workflows that help illustrate sensitivities to material data.

S13: Thermal Transport in Functional Materials and Devices

Thermal Transport

Room: Cypress C

Session Chair: Brian Foley, Georgia Institute of Technology

4:00 PM

(EMA-S13-001-2020) Experimental and Computational Advances in Thermal Boundary Conductance and Nanoscale Thermal Transport across Solid Interfaces (Invited)

A. Giri^{*1}; P. E. Hopkins²

1. University of Virginia, USA
2. University of Virginia, Mechanical and Aerospace Engineering, USA

Interfacial thermal resistance is the primary impediment to heat flow in materials and devices as characteristic lengths become comparable to the mean-free-paths of the energy carriers. This thermal boundary conductance across solid interfaces at the nanoscale can affect a plethora of applications. I will summarize the recent experimental and computational advances that have led to significant atomistic insights into the nanoscopic thermal transport mechanisms at interfaces between various types of materials. I will focus on discussions of works that have pushed the limits to interfacial heat transfer and drastically increased our understanding of thermal boundary conductance on the atomic and nanometer scales near solid/solid interfaces. Specifically, the role of localized interfacial modes on the energy conversion processes occurring at interfaces is emphasized in this review. I will also focus on experiments and computational works that have challenged the traditionally used phonon gas models in interpreting the physical mechanisms driving interfacial energy transport. Finally, I will discuss the future directions and avenues of research that can further our knowledge of heat transfer across systems with broken symmetries.

4:30 PM

(EMA-S13-002-2020) Elimination of Extreme Boundary Scattering via Polymer Thermal Bridging in Silica Nanoparticle Packings

B. F. Donovan^{*1}; R. Warzoha¹; R. Venkatesh²; D. Lee²

1. United States Naval Academy, USA
2. University of Pennsylvania, USA

In this work, we explore thermal transport mechanisms in disordered packings of amorphous nanoparticles with and without a polymer filling the interstices in order to quantify the impact of thermal boundary scattering introduced at nanoparticle edges in an already amorphous system and within the context of a minimum thermal conductivity approximation. By fitting a modified minimum thermal conductivity model to temperature-dependent measurements of thermal conductivity from 80 K to 300 K, we find that the interstitial polymer eliminates boundary scattering in the disordered nanoparticle packing, which surprisingly leads to an increase in the overall thermal conductivity of the disordered nanoparticle thin-film composite. This is contrary to our expectations relative to effective medium theory and our understanding of a minimum thermal conductivity limit. Instead, we find that a stiff interstitial material improves the transmission of heat through a nanoparticle boundary, improving the thermal properties of disordered nanoparticle packing. We expect these results to provide insight into the tunability of thermal properties in disordered solids that exhibit already low thermal conductivities through the use of nanostructuring and vibrational thermal bridging.

4:45 PM

(EMA-S13-003-2020) Atomistic approach to interfacial heat transport phenomenonS. Hosseini^{*1}; S. Nimmala²; E. Lenz²; A. Greaney¹

1. University of California, Riverside, Mechanical Engineering, USA
2. Lam Research, USA

The interaction of heat flow with material interfaces is of increasing technological importance in a variety of fields of electronics where thermal management has become problematic as shrinking device has led to increased heating, but also an increase in interfaces that scatter heat carriers. Theoretical predictions using the conventional Acoustic Mismatch Model (AMM) and Diffusive Mismatch Model (DMM) simplify phonon-interface coupling to extreme cases of fully acoustic and fully diffusive scattering. In this project we modified these conventional methods to include modal properties of phonons in AMM model and phonon occupancy at the interface in DMM model. The transmission coefficient acquired using these models are used to find interfacial thermal conductance using the modified nonequilibrium Landauer equation. The model is further used to characterize the effect of mass, stiffness and lattice mismatch on heat transfer at the interface. We also modeled the scattering coupling at the interface using Fermi golden rule and the results are compared with the former described models. These results are validated against non-equilibrium molecular dynamics simulations using the reverse Müller-Plathe perturbation.

5:00 PM

(EMA-S13-004-2020) Electron and Phonon Thermal Conductance in Ultra-thin (< 40 nm) Ge₂Sb₂Te₅ Layers in Phase Change Memory DevicesK. Aryana^{*1}; J. Nag²; M. Grobis²; J. Read²; J. Gaskins³; D. Olson¹; E. Hoglund¹; J. Howe¹; P. E. Hopkins³

1. University of Virginia, USA
2. Western Digital, USA
3. University of Virginia, Mechanical and Aerospace Engineering, USA

We report on the thermal properties of Ge₂Sb₂Te₅ (GST), commonly used in phase change memory (PCM) devices, at material length scales similar to those used in active memory cells over a wide range of temperatures (25-400 °C). Here, we demonstrate how one can prevent leakage of heat from the electrodes by merely manipulating the boundary conductance. In this regard, we chose tungsten as the electrode and identified that by simply decreasing its thickness, the resistance across the W/GST/W increases up to 40% at elevated temperature (>150 °C). Additionally, we use a series resistor model to measure thermal boundary conductance (TBC) of buried interfaces, in particular, between GST and different spacer compositions (W, SiO₂, and SiNx) which are commonly used in PCM devices. According to our measurements, GST changes phase from amorphous to cubic structure at 150 °C and from cubic to hexagonal at 320 °C. Additionally, the sound speed of GST is obtained by using picosecond ultrasonic measurements and is found to be approximately 2900 m/s for thicknesses below 40 nm.

S14: Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics**High-throughput Approaches/Data Analytics I**

Room: Magnolia B/C

Session Chair: Sergey Levchenko, Skolkovo Institute of Science and Technology

10:00 AM

(EMA-S14-016-2020) Knowledge-Based Approaches in Catalysis and Energy Modelling (Invited)K. Reuter^{*1}

1. Technical University of Munich, Germany

Reflecting the general data revolution, knowledge-based methods are now also entering theoretical catalysis and energy related research with full might. Automatized workflows and the training of machine learning approaches with first-principles data generate predictive-quality insight into elementary processes and process energetics at undreamed-of pace. Computational screening and data mining allows to explore these data bases for promising materials and extract correlations like structure-property relationships. At present, these efforts are still largely based on highly reductionist models that break down the complex interdependencies of working catalyst and energy conversion systems into a tractable number of so-called descriptors, i.e. microscopic parameters that are believed to govern the macroscopic function. For certain classes of materials like transition metal catalysts, corresponding human-designed models have indeed established trend understanding and spurred a targeted materials design. Future efforts will concentrate on using artificial intelligence also in the actual generation and reinforced improvement of the reductionist models. In this talk, I will briefly survey these developments, providing examples from our own research, in particular on adsorption energetics at bimetallic catalysts and data mining for the design of organic semiconductors.

10:30 AM

(EMA-S14-017-2020) Modeling Surface Oxide Growth from First-Principles, Thermodynamics, and Machine Learning (Invited)T. Qiu¹; R. Wexler¹; A. M. Rappe^{*1}

1. University of Pennsylvania, Chemistry, USA

Ab initio thermodynamics has been the method of choice for computationally determining the surface phase diagram of a material under different conditions. The surfaces considered for these studies are often human-selected and too few in number, leading both to insufficient exploration of all possible surfaces and to biases toward portions of the phase space that often do not encompass the most stable surfaces. To overcome these limitations and automate the discovery of realistic surfaces, we combine density functional theory and grand canonical Monte Carlo (GCMC) into "ab initio GCMC." We demonstrate this for the study of oxide overlayers on Ag(111), which, for many years, mystified experts. Ab initio GCMC rediscovers the surface phase diagram with no preconceived notions about the system. Using nonlinear, random forest regression, we discover that Ag coordination number with O and the surface O-Ag-O angles are good descriptors of the energy. Using the evolution histories produced by ab initio GCMC, we deduce a mechanism for the formation of oxide overlayers based on the Ag₃O₄ pyramid motif common to many reconstructions of Ag(111). Ab initio GCMC is a promising tool for the discovery of realistic surfaces that can then be used to study phenomena on complex surfaces, enabling insightful interpretations of experiments.

11:00 AM

(EMA-S14-018-2020) Open Science Platform for Materials Informatics: AiiDA and Materials Cloud (Invited)

F. F. Ramirez*¹

1. EPFL, STI, Switzerland

In recent years, “materials by design” has become a very powerful approach, but it requires running large numbers of simulations on HPC supercomputers and building databases of computed properties. Key challenges are the need to automatically prepare, execute and monitor workflows of calculations, guarantee reproducibility, facilitate data querying and analysis, and share the results. In this talk, we describe our Open Science Platform developed by the Swiss MARVEL NCCR and the European MaX Centre of Excellence, based on the following three pillars. (1) Widely-used, community-based open-source simulation engines. (2) The AiiDA materials informatics infrastructure, to manage, persist, share and reproduce complex computational workflows by automatically tracking the full provenance of data and calculations. (3) The Materials Cloud web platform, to enable the seamless sharing and dissemination of resources in computational materials science: educational, research, and archiving tools; simulation software and services; and curated and raw data. We describe our infrastructure and show examples of how it implements a materials informatics platform supporting researchers in high-throughput computational materials science. We acknowledge the contribution to this work by the entire AiiDA and Materials Cloud teams.

11:30 AM

(EMA-S14-019-2020) Machine Learning Based Predictions of 4f and 5d Electron Binding Energies in Lanthanide-doped Compounds for Novel Scintillator Discovery (Invited)

G. Pilania*¹; A. Talapatra¹; C. Stanek¹; B. P. Uberuaga¹

1. Los Alamos National Laboratory, Materials Science and Technology Division, USA

In many areas in which radiation detection and imaging is required, a key component of the detector system is the scintillating material. However, almost universally, the scintillator is chosen off-the-shelf, without any special consideration for the system at hand. We propose that, by combining experiments with first-principles calculations and machine learning (ML), we can optimize materials for the given application, enhancing properties that are critical at the expense of others that may be less important. This talk will specifically focus on the ML-enabled screening approach of this project in which we build physics-informed statistical learning models to predict electronic binding energies in 4f and 5d levels of lanthanide dopants—primarily responsible for scintillation light yield—in wide bandgap materials. This provides invaluable information for down-selecting materials for further experimental interrogation. ML predictions combined with electronic structure computations and experiments lead to an integrated approach capable of providing both new insights into what drives performance in these scintillators and optimizing them for a specific application.

12:00 PM

(EMA-S14-020-2020) Machine Learning for Chemical Properties and Materials (Invited)

S. Tretiak*¹

1. Los Alamos National Lab, Theoretical Division, USA

Computer simulation is foundational to modern theoretical chemistry. These calculations must be fast and accurate to allow for high-throughput studies of small molecules or the simulation of large systems of many thousands of atoms. Traditional methods are based on classical physics or quantum mechanical (QM) methods. Classical techniques are computationally efficient but have questionable accuracy when used outside of their direct parametrization sets. QM based methods tend to be more accurate than their classical

counterparts, however, their computational scaling is frequently prohibitively expensive to treat realistic systems. Machine learning-based (ML) QM property predictors are capable of fitting directly to QM data with low error while remaining computationally as fast as classical techniques. We present our work on developing and applying various models for QM property prediction, which are trained to large QM datasets then shown to generalize well outside of the training set. The targeted properties include ground state potential energy and forces, various atomic charge schemes, dipoles and quadruples, Infrared spectra, reduced Hamiltonians and a single model for singlet and triplet state energies and forces. Our results show the applicability of these property predictors to systems many times larger than those in the training set with a several magnitude speedup over reference QM methods.

High-throughput Approaches/Data Analytics II

Room: Magnolia B/C

Session Chair: Payam Kaghazchi, Forschungszentrum Jülich GmbH

2:00 PM

(EMA-S14-021-2020) Subgroup Discovery Data Analytics Approach to Catalyst Design

S. Levchenko*¹

1. Skolkovo Institute of Science and Technology, Russian Federation

A reliable prediction of catalytic performance requires understanding and modelling the full catalytic cycle, which is currently not feasible for many materials. A way out is to find indicators for catalytic activity, i.e., common features of good catalysts. In this work, we show how the subgroup discovery (SGD) data-analytics approach [1], combined with ab initio calculations and experimental data, can be used to identify subgroups of materials that optimize a given indicator. As an example, we consider several physically motivated indicators for CO₂ activation, including the OCO bending angle and the C-O bond length l(C-O) in the adsorbed CO₂ molecule. SGD is used to identify subgroups of adsorption sites that provide a small OCO angle or a large l(C-O). Overall, 141 surfaces of 71 different binary and ternary oxide materials are used to find descriptors of the subgroups. Interestingly, for the l(C-O) subgroup all experimentally tested materials are good CO₂-conversion catalysts. The longer l(C-O) is achieved due to the binding of an O atom in the adsorbed molecule to a nearby surface cation, which provides an additional mechanism for weakening C-O bonds. Based on these findings, we propose a set of promising new catalysts for CO₂ conversion.

2:15 PM

(EMA-S14-022-2020) A Machine Learning Study of Magnetism in Actinides

A. Ghosh*¹; F. Ronning²; S. Nakhmanson¹; J. Zhu²

1. University of Connecticut, Materials Science and Engineering, USA

2. Los Alamos National Laboratory, USA

Actinide- and lanthanide-based materials provide an important playground to explore exotic properties stemming from itinerant or localized f-electrons. In particular, uranium-based compounds exhibit emergent phenomena, including magnetism, unconventional superconductivity, hidden order, and heavy fermion behavior. Among them, magnetic properties, such as different orderings of magnetic moments as well as their sizes, are sensitively dependent on pressure, chemical doping and magnetic field due to the strong-correlation effects on 5f-electrons. This presentation will illustrate how regression-based algorithms can be used to identify important material features and construct various machine learning models built on both computational (DFT-simulations) and experimental datasets --- in order to predict magnetic moment size and ordering of actinide systems. This work was supported by the U.S. DOE National Nuclear Security Agency through the LANL LDRD Program and the Institute of Materials Sciences at LANL.

2:30 PM

(EMA-S14-023-2020) Machine learning of octahedral tilting in oxide perovskitesS. R. Xie^{*1}; P. L. Kotlarz¹; J. C. Nino¹; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA

The steady growth of online materials databases, coupled with efforts in materials informatics, has invited the reexamination of existing empirical models through the lens of modern machine learning techniques. Inspired by recent efforts by Bartel et al. to improve on the Goldschmidt tolerance factor for perovskite formation, we apply the Sure Independence Screening and Sparsifying Operator (SISSO) framework to the problem of predicting octahedral tilting. In addition to its impact on the crystal structure, octahedral tilting is related to functional properties, including dielectric permittivity, ferroelectricity, magnetic properties, and metal-insulator transitions. By relating a selection of physical parameters (e.g., atomic radii, electronegativity) with mathematical operations (e.g., addition, exponentiation), we identify an analytical equation that correctly predicts the octahedral tilting classification in a dataset of 60 perovskite oxides with 85% accuracy. Using the same training dataset, we additionally fit and compare seven models generated by other common machine learning methods. Despite the increased complexity afforded by support vector machines, decision trees/random forests, and artificial neural networks, we find that our equation outperforms the other models as well as the original tolerance factor in predicting octahedral tilting.

2:45 PM

(EMA-S14-024-2020) High-Throughput Screening for Identification of Photocathode MaterialsJ. T. Paul^{*1}; A. Galdi²; S. Karkare³; H. Padmore⁴; I. Bazarov²; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA
2. Cornell University, Cornell Laboratory for Accelerator Based Sciences and Education, USA
3. Arizona State University, Physics, USA
4. Lawrence Berkeley National Laboratory, USA

Photocathode brightness is a key parameter in determining the performance of several types of machines, such as Free Electron Lasers (FELs). One avenue of improving this performance is using a photocathode with a lower mean transverse energy (MTE). To identify candidate materials suitable for generating bright electron beams, we screen the MaterialsProject database and perform density-functional theory calculations to determine photoemission properties. We narrow down the number of candidates from tens of thousands of crystals to a subset which are most likely to be excellent photocathode materials. We start with screening based on data available in the MaterialsProject database, such as thermodynamic stability, bandgap, location of the valence band maximum, and effective mass. Next, we re-optimize the crystal structure and calculate the electronic band structure to obtain a more accurate effective mass. To further reduce the number of candidate materials, we calculate their ionization potentials, determine optical transition probabilities, and identify the potential for total internal reflection of electrons. Finally, we calculate the effective mass for the excited states which would emit electrons, estimate the MTE of these crystals, and provide a shortlist of crystals that are likely to have excellent performance as photocathodes and thus improve the design of electron source lasers.

3:00 PM

(EMA-S14-025-2020) K-Means Clustering Analysis of Reflection High Energy Electron Diffraction Data on Epitaxially Grown Oxide Thin FilmsS. R. Provence^{*1}; S. Thapa¹; M. Blanchet¹; T. Truttmann²; B. Jalan²; R. B. Comes¹

1. Auburn University, Dept. of Physics, USA
2. University of Minnesota, USA

Reflection high energy electron diffraction (RHEED) is a robust in situ technique for monitoring epitaxial film deposition. Analysis of RHEED data across the entirety of a deposition is often limited to using a few snapshots during the deposition to provide qualitative information about the growth or measuring the change in intensity of one or a few spots to monitor RHEED oscillations. Machine learning algorithms may provide a more quantitative approach to extracting information from RHEED patterns across the entirety of a growth. A data pipeline for analysis of a full RHEED video is developed using principle component analysis (PCA) to compress the data into the components with the most statistical variance in the data set. K-means clustering is used to provide time domain boundaries on positions observed in the RHEED patterns during oxide thin film depositions. A series of thin oxide films grown using hybrid oxide molecular beam epitaxy (hMBE) is analyzed by segmenting the growth into clusters corresponding to phases of the deposition. An analysis of the time intervals of the clusters can be used to help understand the time evolution of the surface structure of these films.

Multiscale modeling

Room: Magnolia B/C

Session Chair: Payam Kaghazchi, Forschungszentrum Jülich GmbH

4:00 PM

(EMA-S14-026-2020) Prediction of oxygen reduction kinetics at fuel cell cathodes: First principles calculations (Invited)E. A. Kotomin^{*1}; R. Merkle¹; Y. Mastrikov²; J. Maier¹

1. Max Planck Institute for Solid State Research, Germany
2. University of Latvia, Institute of Solid State Physics, Latvia

The efficiency of solid oxide fuel cells (SOFC) depends critically on materials, especially, for the cathode where the oxygen reduction reaction (ORR) occurs. We will discuss the results of large scale first principles calculations for the two alternative polar --(La,Sr)O and MnO₂ (001)-- terminations of (La,Sr)MnO₃ cathode materials. Surface oxygen vacancy and oxygen adsorbate concentrations strongly depend on the Mn oxidation state, and surface polarity. It is shown that the surface oxygen vacancy concentration on the (La,Sr)O termination is five orders of magnitude smaller compared to MnO₂, which (despite higher oxygen adsorbate coverage) leads to drastically decreased estimated ORR rates. Similar results have recently also been obtained by the first principles calculations for (La,Sr)CoO₃. Thus, it is predicted for both prototypical SOFC cathode materials that the BO₂ termination largely determines the ORR kinetics, although with Sr surface segregation (long-term degradation) its fraction of the total surface area decreases which slows down cathode kinetics.

4:30 PM

(EMA-S14-027-2020) Manufacturing of Lithium Ion Batteries from a Multiscale Modeling Perspective (Invited)A. A. Franco^{*1}

1. Université de Picardie Jules Verne, LRCS, France

In this lecture I report recent research progress achieved in our ARTISTIC project, which aims at developing a multiscale computational platform simulating the different steps along the fabrication process of Lithium Ion Batteries (LIB). Such a platform aims at predicting the influence of the process parameters

on the final LIB performance upon cycling, but also at performing reverse engineering. The platform combines physical models (e.g. Coarse Grained Molecular Dynamics, Discrete Element Method, continuum) with Artificial Intelligence algorithms devoted to the models parameterization but also to the analysis of the experimental data. Results are presented in regards to the simulation of slurries, coating, drying, calendaring and electrolyte impregnation for different NMC-based formulations. Furthermore, 4D-resolved continuum performance simulations capturing the influence of the spatial location of carbon-binder within the electrodes on the electrochemical response are also discussed. The practical implications of the ARTISTIC platform towards the fabrication process optimization and the integration of new battery chemistries are discussed.

5:00 PM

(EMA-S14-028-2020) Shape-Selective Growth of Nanoscale Materials: Insights From Multi-Scale Theory and Simulation (Invited)

K. Fichthorn*¹

1. Pennsylvania State University, Chemical Engineering, USA

A significant challenge in the development of functional nanomaterials is understanding the growth of colloidal metal nanocrystals. Despite ample demonstrations that it can be highly beneficial to tune nanocrystal morphologies for specific applications, it is still difficult to achieve high, selective yields in most synthesis protocols. Many fundamental aspects of these complex syntheses remain poorly understood. Our multi-scale theoretical studies based in quantum density-functional theory (DFT) highlight how various nanocrystal shapes can be governed by either thermodynamics or kinetics. We use a variety of classical molecular-dynamics (MD) simulation techniques based on our many-body force field to show that the growth of sufficiently large Ag nanocubes with PVP capping molecules is induced by the facet-selective deposition kinetics of solution-phase Ag atoms/ions. When chloride is introduced to the synthesis, Ag nanocubes grow with a thermodynamic driving force. Fivefold-twinned Ag nanowires grow by surface diffusion induced by the unique, strained structure of these fascinating objects. I will also discuss the growth of fivefold-twinned Cu nanowires in the presence of chloride and HDA, where DFT calculations indicate that growth is dominated by deposition kinetics. These scenarios indicate the various pathways to achieve shape-selective syntheses in the future.

S16: Molecular, Inorganic, and Hybrid Ferroelectrics for Optoelectronic and Electronic Applications

Metal-organic Halide Perovskites

Room: Citrus B

Session Chair: Lauren Garten, U.S. Naval Research Lab

2:00 PM

(EMA-S16-001-2020) Theory and modeling of correlated ionic and electronic motions in hybrid organic-inorganic perovskites (Invited)

A. Kakekhani¹; A. M. Rappe*¹

1. University of Pennsylvania, Chemistry, USA

The perovskite crystal structure hosts a wealth of intriguing properties, and the renaissance of interest in halide (and hybrid organic-inorganic) perovskites (HOIPs) has further broadened the palette of exciting physical phenomena. Breakthroughs in HOIP synthesis, characterization, and solar cell design have led to remarkable increases in reported photovoltaic efficiency. However, the observed long carrier lifetime and PV performance have eluded comprehensive physical justification. The hybrid perovskites serve as an enigmatic crossroads of physics. Concepts from crystalline band

theory, molecular physics, liquids, and phase transitions have been applied with some success, but the observations of HOIPs make it clear that none of these conceptual frameworks completely fits. In this talk, recent theoretical progress in understanding HOIPs will be reviewed and integrated with experimental findings. The large amplitude motions of HOIPs will be highlighted, including ionic diffusion, anharmonic phonons, and dynamic incipient order on various length and time scales. The intricate relationships between correlated structural fluctuations, polar order, and excited charge carrier dynamics will also be discussed.

2:30 PM

(EMA-S16-002-2020) Electronic structure of the Ruddlesden-Popper analogs of methylammonium lead iodide

B. Phan*¹; S. R. Xie¹; P. Li²; S. R. Phillpot¹; R. G. Hennig¹

1. University of Florida, Materials Science and Engineering, USA

2. Wuhan University of Science and Technology, China

We explore the stability and electronic structure of the Ruddlesden-Popper (RP) phases for methylammonium lead iodide, a hybrid organic-inorganic perovskite, $\text{An}+1\text{BnX3n}+1$, with $\text{A}=\text{CH}_3\text{NH}_3$, $\text{B}=\text{Pb}$, $\text{X}=\text{I}$. RP phases are layered relatives of the perovskite structure, consisting of perovskite slabs separated by rock salt layers. In this work, we determine the thermodynamic stability, band gap, and carrier effective masses of the $(\text{CH}_3\text{NH}_3)_{n+1}\text{PbnI3n}+1$ RP series using density functional theory. These properties are affected by our choice of functional (PBE, SCAN, and HSE06) and the inclusion of van der Waals corrections and spin-orbit coupling. We compare the relative stability of the different RP orders in $(\text{CH}_3\text{NH}_3)_{n+1}\text{PbnI3n}+1$ and $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n}+1$, an extensively-studied inorganic RP series. We show that this materials class has a tunable band gap in the visible light range, where the band gap increases with n . The results indicate that the hybrid organic-inorganic RP phases can be synthesized and are potentially useful for optoelectronic and energy applications.

2:45 PM

(EMA-S16-003-2020) Tomographic Nano-Photovoltaic Properties of Halide Perovskites

J. Song*¹; W. Linthicum¹; Y. Zhou²; B. Huey¹

1. University of Connecticut, Materials Science and Engineering, USA

2. Brown University, School of Engineering, USA

Halide Perovskites such as MAPbI_3 have become the most highly investigated materials system of the century, due to its superlative photovoltaic properties leading towards potential applications as low cost solar cells, light sensors, light emitting diodes, and lasers. Scanning Probe Microscopy is an obvious tool for mapping any nanoscale variations in these typically polycrystalline thin films, including Scanning Surface Potential Microscopy, PhotoConductive AFM, and even Tomographic AFM. Combining these methods, the importance of grains, grain boundaries, and triple junctions are directly mapped, throughout the thickness of MAPbI_3 photoconductors. Work function differences, grain size dependencies, and effective mean free paths for photocarriers are also revealed from the nanoscale-resolved volumetric results.

3:00 PM

(EMA-S16-004-2020) Ferroelectric poling of methylammonium lead iodide thin-films

H. Röhm¹; T. Leonhard¹; M. J. Hoffmann¹; A. Colmann*¹

1. Karlsruhe Institute of Technology, Material Research Center for Energy Systems, Germany

Among the emerging photovoltaic technologies, perovskite solar cells stand out with remarkable power conversion efficiencies and low-cost solution processability, rivaling established technologies. Seemingly contradictory reports on polar domains and their origin have surrounded the controversial discussion about the

ferroelectricity of the methyl ammonium lead iodide (MAPbI₃) thin-films that are commonly employed in perovskite solar cells. In this work, microscopic modulations of the polar domain patterns upon application of an electric poling field are correlated with macroscopic changes to the currents through the MAPbI₃ layer. Piezoresponse force microscopy is used to monitor the widening, narrowing, generation or extinction of polar domains as well as shifts of the domain walls under an in-plane electric poling field that is applied between two laterally organized electrodes. This poling leads to a net polarization of individual grains and the thin-film itself. Macroscopically, this net polarization results in a persistent shift of the diode characteristics that was measured across the channel between the electrodes. Both, the modulation of the polar domains upon electric poling as well as the concurrent persistent shift of the electric currents through the device are the unambiguous hallmarks of ferroelectrics, which evidences that MAPbI₃ is a ferroelectric semiconductor.

Beyond Metal-organic Halide Perovskites

Room: Citrus B

Session Chair: Alexander Colsmann, Karlsruhe Institute of Technology

3:45 PM

(EMA-S16-005-2020) Ferroelectric Inorganic Perovskite Oxides for Photovoltaic Applications (Invited)

T. Fix*¹

1. CNRS and University of Strasbourg, ICube, France

Ferroelectric (FE) materials are under intense scrutiny for photovoltaic applications (PV), following the demonstration of above 8% conversion efficiency in FE-based solar cells. In these cells, there is no need for a p-n junction because the electric polarization from ferroelectricity is responsible for the current flow. The key issue for the development of oxide absorbers for PV is their bandgap that is generally above 3 eV. In this work, we produced Bi₂FeCrO₆ (BFCO) oxide materials by pulsed laser deposition (PLD). The structural, optical and electrical properties are presented. High quality epitaxial growth and phase-pure films are demonstrated by X-ray diffraction. We have studied the evolution of parameters such as the bandgap versus the growth conditions, proving that it can be adjusted from 1.9 to 2.6 eV. Resonant X-ray diffraction is performed at ESRF to investigate the origin of the variation of the bandgap. The ferroelectric properties are investigated by piezoresponse force microscopy (PFM). We observe that light influences the state of polarization of BFCO. Finally, devices based on BFCO are fabricated and their photovoltaic properties are analysed.

4:15 PM

(EMA-S16-006-2020) All-oxide heterostructures based on solution-processed ferroelectric photoabsorbers for PV (Invited)

P. Machado¹; I. Caño¹; M. Scigaj¹; M. Coll*¹

1. ICMAB-CSIC, Superconducting Materials and Large Scale Nanostructures, Spain

The use of ferroelectric perovskite oxides as a stable photoactive layer has opened up a ground-breaking new arena of research. They present an alternative mechanism for solar energy conversion that could surpass the fundamental efficiency limits of conventional semiconductors. One of the biggest challenges so far is to reduce their band gap toward the visible region while simultaneously retaining ferroelectricity. To address these two issues, we perform elemental composition engineering of BiFeO₃ as a means to tune the characteristics of the cation-oxygen bonds and gain new insights on its influence on the structure, optical and electronic properties by means of XRD, spectroscopic ellipsometry, photoemission and X-ray absorption spectroscopy. We demonstrate by chemical deposition techniques the formation of epitaxial pure-phase, and stable

co-substituted BiFeO₃ films. The band gap can be tuned from 2.7 to 2.3 eV upon transition metal substitution while simultaneously enhancing ferroelectricity [1]. A-site substitution by lanthanides can further modify the optical absorption while increasing film reproducibility at high Co-loads. Finally, non-optimized all-oxide vertical devices have been fabricated and the electrical photoresponse in the visible regions in co-substituted films is improved with respect to undoped BiFeO₃.

4:45 PM

(EMA-S16-007-2020) Tunable quadruple-well ferroelectric van-der-Waals crystals (Invited)

S. M. Neumayer¹; J. A. Brehm¹; L. Tao²; A. O'Hara³; M. Susner²; M. McGuire¹; P. Ganesh¹; S. T. Pantelides³; P. Maksymovych¹; N. Balke Wisinger*¹

1. Oak Ridge National Lab, USA
2. Air Force Research Lab, USA
3. Vanderbilt University, Dept. of Physics and Astronomy, USA

The family of layered thio- and seleno-phosphates has gained attention as possible control dielectrics for the rapidly growing family of 2D and quasi-2D electronic materials. Here we report a combination of density-functional-theory (DFT) calculations, DFT-based molecular-dynamics (MD) simulations, and variable-temperature, -pressure, and -bias piezoresponse force microscopy (PFM) data to predict and verify the existence of an unusual ferroelectric property – a uniaxial quadruple potential well for Cu displacements – enabled by the van-der-Waals (vdW) gap in ferroelectric copper indium thio-phosphate (CuInP₂S₆). The calculated potential-energy landscape for Cu displacements is strongly influenced by strain, accounting for the origin of the giant negative piezoelectric coefficient. Experimental data verifies the co-existence of four polarization states which show complex ferroelectric switching pathways which are supported by bias-dependent MD simulations. The combined theory-experiment approach also allows to map strain and stress in the material on the length scales of 10's of nm using PFM. These phenomena offer new opportunities for both fundamental studies and applications in data storage and electronics.

5:15 PM

(EMA-S16-008-2020) Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods

K. Choudhary*¹

1. National Institute of Standards and Technology, MML, USA

Solar energy plays an important role in solving serious environmental problems and meeting the high energy demand. However, the lack of suitable materials hinders further progress of this technology. Here, we present the largest inorganic solar cell material search till date using density functional theory (DFT) and machine-learning approaches. We calculated the spectroscopic limited maximum efficiency (SLME) using the Tran-Blaha-modified Becke-Johnson potential for 5097 nonmetallic materials and identified 1997 candidates with an SLME higher than 10%, including 934 candidates with a suitable convex-hull stability and an effective carrier mass. Screening for two-dimensional-layered cases, we found 58 potential materials and performed G₀W₀ calculations on a subset to estimate the prediction uncertainty. As the above DFT methods are still computationally expensive, we developed a high accuracy machine-learning model to prescreen efficient materials and applied it to over a million materials. Our results provide a general framework and universal strategy for the design of high-efficiency solar cell materials. The data and tools are publicly distributed at: <https://www.ctcms.nist.gov/~knc6/JVASP.html>, <https://www.ctcms.nist.gov/jarvis/ml/>, <https://jarvis.nist.gov/>, and <https://github.com/usnistgov/jarvis>.

Friday, January 24, 2020

S4: Complex Oxide Thin Film Materials **Discovery: From Synthesis to Strain/Interface** **Engineered Emergent Properties**

Novel Synthesis Techniques

Room: Orange A

Session Chair: Christina Rost, University of Virginia

9:30 AM

(EMA-S4-033-2020) Exploring the Interplay Between Structure, Charge, and Spin in Entropy-Stabilized Oxides (Invited)

J. Heron^{*1}

1. University of Michigan, USA

Entropy-stabilized oxides (ESOs) demonstrate a new and unprecedented degree of chemical control in materials. The technique can be used to incorporate cationic species in an atypical coordination, such as Cu²⁺ and Zn²⁺ into octahedral coordination and increase the solubility of elements. This broadens the compositional space of crystalline oxides and presents opportunities to understand and explore the local chemical and structural disorder resulting from different atomic sizes and the preferred coordination of the constituents. Particularly in oxides, where the physical behavior is strongly correlated to stereochemistry and electronic structure, entropic stabilization creates a unique platform to tailor the interplay between structural and chemical disorder to realize unprecedented functionalities. Here, I will discuss our recent results that investigate the magnetic and dielectric properties of single crystalline (MgCoNiCuZn)O thin films using exchange coupling in thin film heterostructures, Xray synchrotron, and DFT. I will discuss our work using compositional variants to explore the interplay between structure, charge, and spin in this system.

10:00 AM

(EMA-S4-034-2020) Tunability of native defect density through local configuration-controlled disorder in entropy-stabilized oxides

S. Chae^{*1}; Z. Wang²; L. Williams¹; S. Novakov⁴; S. Sung¹; P. B. Meisenheimer¹; R. Hovden¹; D. Schlom³; E. Kioupakis¹; J. Heron⁴

1. University of Michigan, Materials Science and Engineering, USA
2. Cornell University, USA
3. Cornell University, Department of Materials Science and Engineering, USA
4. University of Michigan, USA

Entropic stabilization has become a strategy to create new oxide materials and novel properties, however, achieving an atomistic understanding of these properties has been challenged by the local compositional and structural disorder that underlies their fundamental structure-property relationships. Here, we combine high-throughput atomistic calculations, machine-learning algorithms, and experimental characterization to investigate the role of local configurational and structural disorder on the thermodynamics of intrinsic point defects in (MgCoNiCuZn)O-based entropy-stabilized oxides (ESOs) and their influence on the electrical properties. From theory, we find that the cation-vacancy formation energy decreases with increasing local tensile strain, while oxygen-vacancy formation depends on the local structural distortion associated with the local configuration of chemical species. Through relatively small changes in the mole fraction of cations, the equilibrium defect density can be tuned by over two orders of magnitude. Vacancies in ESOs exhibit deep thermodynamic transition levels leading to transport via variable range hopping. Our results motivate tuning local structural distortions by local alloy composition as an engineering principle to enable controlled defect formation in multi-component oxides.

10:15 AM

(EMA-S4-035-2020) Growth and Dielectric Characterization of Epitaxial Entropy-Stabilized Oxide Thin Films

G. N. Kotsonis^{*1}; J. Maria¹

1. The Pennsylvania State University, Materials Science and Engineering, USA

At elevated temperatures, entropy-stabilized oxide (ESO) phases (such as the prototype composition Mg_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2}O) stabilize in a crystalline solid-solution that is typically quenched for characterization. Low temperature metastability leads to microstructure and property dependences on thermal history and synthesis kinetics. In particular, ESO optical constants at visible wavelengths depend appreciably on composition, thin film growth conditions (e.g. substrate temperature), and post-growth heat treatments. To illustrate these dependences, we present structural and optical characterization of epitaxial Mg_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2}O and related compositions as a function of thin film growth conditions and post-deposition heat treatments. The large compositional solubility ranges available to ESO systems provide an avenue for physical property tuning in ESO systems, if trends linking properties, composition, and synthesis conditions can be understood and controlled.

10:30 AM

(EMA-S4-036-2020) Atomic Layer Deposition: From molecular chemistry to nanocoatings of functional complex oxides

P. Yu¹; C. Bohr²; S. Beer³; S. Mathur²; A. Devi³; M. Coll^{*1}

1. ICMAB-CSIC, Superconducting Materials and Large Scale Nanostructures, Spain
2. University of Cologne, Institute of Inorganic Chemistry, Germany
3. Ruhr-University Bochum, Inorganic Chemistry, Germany

Preparation of functional oxide thin films at low temperature, over large areas and compatible with low- cost and flexible substrates, offers great industrial potential. Atomic layer deposition (ALD) is unique chemical thin-film deposition method because it ensures excellent large-area uniformity, conformality, and enables simple and atomic level control of film thickness and composition. Additionally, ALD favors controlling and nanoengineering of interfaces and conformal coatings of 3D substrates. The precursor chemistry is one of the main parameters that determines the processing conditions and ultimately the film properties. Despite commercially available ALD precursors, there is an increasing need for new or improved precursors to further enrich the variety of ALD functional oxides, especially multicomponent oxides. Here we explore for the first time the use of a single-source heterobimetallic precursor versus multiple-source precursors to stabilize Gd-Fe-O thin films, attractive for its potential applications in magneto-optical devices. The influence of ligand moieties and ALD process design on the stoichiometry, morphology, film structure and phase purity of the deposited films is studied by means of XPS, SEM and XRD characterization techniques, respectively.

10:45 AM

(EMA-S4-037-2020) Asynchronously Patterned Pulsed Sputtering (APPS) of Complex Materials from Elemental Targets

T. M. Borman^{*1}; M. D. Hossain¹; J. Hayden¹; J. Maria¹

1. Pennsylvania State University, Materials Science and Engineering, USA

The authors describe a new technique, asynchronously patterned pulsed sputtering (APPS), for deposition of complex materials using multiple High Power Impulse Magnetron Sputtering (HiPIMS) sources. A key advantage of HiPIMS (relative to DC or RF sputtering) is the decoupling of deposition rate from energetics. However, when co-sputtering with multiple HiPIMS sources, some of this freedom is lost. If operated at different frequencies (allowing independent flux control) some pulses occur at different times while others overlap. This can result in a plasma which is variable from pulse to pulse. Alternatively, if the rate of the pulses is synchronized,

independent control of rate and energetics is lost as voltage and pulse width are now used to control rate. APPS consists of one source running at a given frequency for every pulse while the second source runs asynchronously at the same frequency, following a pattern of pulses and skips. By changing the ratio of pulses to skips, the relative fluxes of the two sources can be controlled. APPS enables deposition within a few atomic percent across the entire composition range from just two deposition rate (flux) measurements, with more precise control from further measurements in regions of interest. The setup and application of APPS to metal alloy and reactive (carbide and oxide) sputtering, will be discussed.

11:00 AM

(EMA-S4-038-2020) Reactively-sputtered GaN using Hi-Power Impulse Magnetron Sputtering

J. Nordlander^{*1}; K. Ferri¹; J. Maria¹; Z. Sitar²; R. Collazo²

1. Pennsylvania State University, USA
2. North Carolina State University, Materials Science and Engineering, USA

In this presentation, we demonstrate that reactive High-Power Impulse Magnetron Sputtering (HiPIMS) is an effective low temperature alternative for depositing high quality, epitaxial GaN thin films. In contrast to conventional direct current (DC) or radio frequency (RF) sputtering, pulsed DC provides the needed kinetic energy and ionization fraction to establish a sufficiently reactive environment to promote full nitridation. This can be challenging with many other Ga sources. More specifically, the low duty cycle regime of pulsed DC known as HiPIMS provides access to kW/cm² peak power densities without target degradation and thus dramatically increased gallium reactivity. In addition, adding an opposite polarity voltage pulse between the target bombarding events, known as a kick pulses, further allows one to tailor both the adatom landing energy on the substrate surface, and mitigate target poisoning. This unique capability set enables us to prepare high crystal quality epitaxial GaN thin films with smooth surface morphologies characterized by c/2 steps and terraces at temperatures below 500 °C. The presentation will focus on the relationships between sputtering parameters including voltage, kick pulse, pulse length, and duty cycle, on GaN thin film crystal quality, surface morphology, and growth rate. Preliminary transport properties will be reported.

S5: Mesoscale Phenomena in Ferroic Nanostructures: Beyond the Thin-Film Paradigm

Modeling, Simulation and Processing

Room: Cypress C

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

8:30 AM

(EMA-S5-001-2020) Mesoscale Modeling of Light Transmission Modulation in Ceramics (Invited)

L. Kuna^{*1}; J. Mangeri²; J. Wollmershauser³; E. Gorzkowski³; S. Nakhmanson⁴

1. University of Connecticut, Physics, USA
2. Institute of Physics, Czech Academy of Sciences, Dielectrics, USA
3. U.S. Naval Research Laboratory, USA
4. University of Connecticut, Materials Science and Engineering, USA

This presentation introduces a novel modeling approach for simulating properties of polycrystalline ceramics with coupled optical, elastic and dielectric degrees of freedom. The approach is implemented in the Ferret application, developed at UConn and built upon the MOOSE framework, a part of the DoE initiative to create high-quality open-source software for scientific computing. Ferret computational capabilities allow for the determination of the

dependency of optical properties on polycrystalline grain orientation, size, and shape, as well as temperature and the action of externally applied electric fields and elastic strains. In particular, we adopt a modification of the wave-retardation theory, developed by Raman and Viswanathan in 1955, for evaluation of optical transmission through a polycrystal, which produces excellent agreement with experimental results obtained for various ceramic materials in both visible and infrared parts of the EM spectrum. Furthermore, our computational approach can also predict the modulation of transmittance under a variety of applied mechanical, electrical and thermal conditions, showing changes from full transparency to opacity in some cases. The results of these investigations highlight a remarkable promise of functional nano- and micro ceramics for a range of advanced engineering applications, including transparent armor, multi-functional IR domes and metamaterials by design.

9:00 AM

(EMA-S5-002-2020) Investigation of Electrostatic Interactions in Ferroelectric-Dielectric Composites at Mesoscale

K. Co¹; L. Kuna²; J. Mangeri³; P. Alpay¹; S. Nakhmanson^{*1}

1. University of Connecticut, Materials Science and Engineering, USA
2. University of Connecticut, Physics, USA
3. Institute of Physics, Czech Academy of Sciences, Dielectrics, Czechia

Ferroelectric-dielectric composite systems display a wide range of phenomena that are attractive for future technological applications, such as enhanced dielectric tunability and energy storage density, multi-state ferroelectric switching, and reduced conductivity and loss. In a system consisting of spherical ferroelectric nanoparticles embedded in a dielectric matrix, adjustment of particle size, spacing, and concentration, alongside the material properties of both the ferroelectric and matrix phases, can produce structures with preprogrammed behavior and novel functionalities. Here we utilize an open-source highly scalable real-space finite-element-method based code Ferret, to study field-induced properties of ferroelectric-dielectric composites. We evaluate the influence of particle size, spacing and the properties of the dielectric matrix on the behavior of a ferroelectric-dielectric composite. The developed insights provide new routes for the design of composite metamaterials whose dielectric properties can be controlled and tuned through altering the morphology and arrangement of their ferroelectric components, as well as the characteristics of the enveloping dielectric.

9:15 AM

(EMA-S5-003-2020) Domain wall variant-engineered dielectric meta-materials (Invited)

J. E. Spanier^{*1}

1. Drexel University, Materials Science & Engineering, USA

Ordering of ferroelectric polarization and its trajectory in response to an electric field are essential for the operation of non-volatile memories, transducers, and electro-optic devices. However, for voltage control of capacitance and frequency, domain walls have long been thought to be a hindrance because they lead to high dielectric loss and hysteresis in response to an applied electric field. To avoid these effects, tunable dielectrics are often operated under piezoelectric resonance conditions, relying on operation well above the ferroelectric Curie temperature, where tunability is compromised. Therefore, there is an unavoidable trade-off between the requirements of high tunability and low loss in tunable dielectric devices, which leads to severe limitations on their figure of merit. In this talk I will discuss our recent re-examination of the ferroelectric polarization-energy landscapes associated with domain walls and their motion. Intrinsically tunable materials exhibit properties that are defined not only by their chemical composition, but also by the proximity and accessibility of thermodynamically predicted strain-induced, ferroelectric domain-wall variants. Starting from application of Ginzburg-Landau-Devonshire theory, under special

conditions we predict and observe high dielectric tunability and the emergence of dynamic behavior that yields low-loss RF microwave resonant responses.

10:30 AM

(EMA-S5-005-2020) Ferroelectric Domain Configurations and Switching Processes for Multiferroic BFO-based Epitaxial Thin Films (Invited)

J. Song¹; Y. Huang²; J. Steffes¹; R. Ramesh²; B. Huey^{*1}

1. University of Connecticut, Materials Science and Engineering, USA
2. University of California, Berkeley, Materials Science and Engineering, USA

Ferroelectric switching is a critical process in the multiferroic systems BiFeO₃ and La-doped BiFeO₃ for potential applications in data storage, magnetoelectric detection, and even beyond-CMOS low-power transistors. The switching process in BFO and LBFO are compared, revealing multistep switching for both systems. The reorganization of ferroelectric domains following 'voltage annealing' of as-prepared domain patterns, notably through the thickness of the epitaxial film according to Tomographic AFM, furthermore provides insight into domain wall energies and stable domain configurations.

11:00 AM

(EMA-S5-006-2020) Phase transformation in amorphous complex oxide films and routes towards epitaxial integration of BiFeO₃ on Si

A. Plokhikh^{*1}; I. Karateev³; M. Falmbigl¹; A. Vasiliev³; J. Lapano²; R. Engel-Herbert²; J. E. Spanier¹

1. Drexel University, Materials Science & Engineering, USA
2. The Pennsylvania State University, Materials Science and Engineering, USA
3. Kurchatov Institute, Russian Federation

Atomic layer deposition (ALD) possesses characteristics that are unachievable by other deposition methods. Unfortunately, use of ALD for producing complex oxides has been limited due to the difficulty of formation of complex crystalline materials by this technique. Reports on the solid-state phase epitaxial transformation of amorphous films have been limited, and our work addresses the challenge in BiFeO₃ films. We demonstrate that amorphous super-structured Bi-Fe-O has clear advantages in terms of composition and growth control, but does not exhibit low-temperature transformation benefits due to interdiffusion limitations. We present on studies showing significantly decreased phase-transformation temperatures enabling epitaxial integration of BiFeO₃ films on Si by implementing well-intermixed Bi-Fe-O on SrTiO₃/Si substrates. The solid-solid transformation of such films was investigated by in situ XRD, TEM and XPS measurements and reveals a very complex crystallization process towards epitaxial integration. It encompasses phenomena such as reorientation, recrystallization, and grain growth which yield the formation of epitaxial BiFeO₃ on Si substrate at temperatures below 400°C. Work supported by ONR under N00014-15-11-2170 and NSF DMR 1420620.

11:15 AM

(EMA-S5-007-2020) Integration of Si(001) with Functional Oxides using Graphene-Oxide Interface Layer (Invited)

M. Spreitzer^{*1}; Z. Jovanovic¹; U. Gabor¹; D. Suvorov¹

1. Jozef Stefan Institute, Advanced Materials, Slovenia

Epitaxial integration of complex oxides with semiconductors is often limited by lattice mismatch between the two material systems and their dissimilar chemical properties. However, in the case of 2D materials, these strict requirements can be alleviated by the weak van der Waals interactions and can allow remote epitaxial registry with a substrate at long distances. In the present work, we investigated

the potential of graphene oxide (GO) to act as a template for pulsed-laser deposition (PLD) growth of SrTiO₃ (STO) on Si(001)/SiO₂ surface. The results revealed that GO can direct the growth of STO to a smooth, compact and pinhole-free layer, with mostly (001) out-of-plane orientation. When this was combined with SrO-assisted deoxidation of silicon surface, a partially epitaxial, highly crystalline STO film, with exclusively (001) out-of-plane orientation, was obtained. Thanks to high-quality, as-grown STO was used as a pseudo-substrate for piezoelectric integration Pb[Zr_{0.52}Ti_{0.48}]O₃ (PZT), that exerted properties comparable to ones obtained in more complex integration methods. Our results suggest that GO can be used as a template for the integration of complex oxides with silicon in a way that is less demanding in terms of interface control and vacuum conditions, which are important advantages for the development of large-area PLD processes.

11:45 AM

(EMA-S5-008-2020) Atomic-scale control of the domain structure, strain and chemistry in BaTiO₃ without the use of contact electrodes (Invited)

M. Barzilay¹; H. Elangoval¹; T. Qiu²; A. M. Rappe²; Y. Ivry^{*1}

1. Technion - Israel Institute of Technology, Department of Materials Science and Engineering / Solid State Institute, Israel
2. University of Pennsylvania, Department of Chemistry, USA

Applying electric fields on ferroelectrics usually requires contact electrodes. However, the use of contact electrodes imposes severe undesired limitations on device miniaturization. We applied electromagnetic fields without the use of contact electrodes, allowing us to controllably form periodic domains with density as high as (2.5 nm)⁻¹, which is promising for domain-wall electronics. We show that by pre-designing the geometry of the ferroelectric, the electromagnetic field can be used to switch the periodic domains controllably as well as to demonstrate a new form of giant electro-mechanical coupling. Lastly, we demonstrate that for strong electromagnetic fields, the interaction with the material can be used to modify the surface chemistry with atomic-scale precision, paving the way to ferroelectric-based nanoscale catalysis and local electro-chemical patterning.

12:15 PM

(EMA-S5-009-2020) Aerosol Deposition and Characterization of Nano-structured Ergodic Relaxor Thick Films (Invited)

E. A. Patterson^{*1}; S. D. Johnson¹; E. Gorzkowski¹; S. E. Veras¹

1. US Naval Research Lab, USA

Aerosol Deposition is a thick-film deposition process that enables rapid production of up to hundreds of micron thick layers of ceramic materials entirely at room temperature. The high-speed impact and fracture of the starting particles results in films with crystallite sizes on the order of 10-20 nm. Ferroelectric materials, such as barium titanate, have highly constrained, nearly linear, hysteresis in such films due to these nano-grained microstructures and high residual stresses. Therefore, bismuth sodium titanate (BNT)-based relaxor ferroelectric compositions were used to take advantage of their inherent nano-polar regions. Films were deposited onto metal substrates (copper, aluminum, steel) to facilitate their electrical characterization. In this work, the processing, deposition, structural, dielectric, and ferroelectric properties of these films are presented.

S6: Complex Oxide and Chalcogenide Semiconductors: Research and Applications

Low Dimensional Systems

Room: Magnolia A

Session Chairs: Ryan Comes, Auburn University; Jayakanth Ravichandran, Columbia University

8:30 AM

(EMA-S6-008-2020) Synthesis and properties of chalcogenide heterostructures with designed nanoarchitecture (Invited)

S. Bauers*¹; D. Roberts¹; A. Zakutayev¹

1. National Renewable Energy Laboratory, USA

2D heterostructures are often prepared by exfoliation and reassembly of individual layers, but this approach is generally limited to materials that can be isolated as freestanding “nanosheets” and is difficult to scale-up for technological adoption. We will discuss chalcogenide heterostructures synthesized by an alternative approach, whereby vapor-deposited thin-films are gently heated to activate self-assembly into multilayered nanocomposites. This allows for integration of constituent layers that cannot be individually isolated, such as 3D crystals terminated by 2D confinement, or emergent 2D phases with no bulk analogue. We will show that heterostructures based on TiSe₂ and VSe₂ have tunable properties through nanoarchitectural control at the level of monolayers. For example, in VSe₂-based structures charge exchange between layers, dimensionality, and defects all affect the onset of a charge-density wave (CDW). Motivated by results in selenide systems, as well as the hysteretic CDW observed in TaS₂, we have recently incorporated this material into heterostructures, marking the first application of this synthesis approach to sulfur-based chemistries. Initial results on TaS₂-based heterostructures demonstrate monolayer control similar to that seen in selenide systems, and act as a promising first step in utilizing these materials for investigation of emergent properties in 2D assemblies.

9:00 AM

(EMA-S6-009-2020) Topological insulator heterostructures: From axions to spintronics (Invited)

N. Samarth*¹

1. Pennsylvania State University, USA

The confluence of fundamental symmetries (such as time reversal invariance) and relativistic quantum mechanics is known to produce emergent electronic states in crystalline solids that are accurately described using the language of topology. This talk discusses how the synthesis and study of topological quantum materials yields a playground for both exotic pursuits at millikelvin temperatures such as axion electrodynamics in condensed matter and pragmatic spintronics technologies that work under ambient conditions. Supported by SMART, one of seven centers of nCORE, an SRC program, sponsored by National Institute of Standards and Technology (NIST), the Penn State Two-Dimensional Crystal Consortium-Materials Innovation Platform (2DCC-MIP) under the U.S. National Science Foundation Grant No. DMR-1539916, and IQM-EFRC funded under U. S. DOE, Basic Energy Sciences, Materials Sciences & Engineering Award DE-SC0019331.

9:30 AM

(EMA-S6-010-2020) Understanding Thermal Expansion in Layered Chalcogenides (Invited)

J. Rondinelli*¹

1. Northwestern University, USA

Ferroelectric perovskite oxides have recently been used in solar applications because their polarity allows for the separation of photocarriers when under illumination to generate a photocurrent.

Oxides, however, often have band gaps that are beyond the solar-optimal regime (>3.3 eV); for this reason, perovskite-structured chalcogenides have been proposed as suitable candidate materials owing to their lower band gaps (≈2 eV). An understanding of the thermal expansion behavior of photovoltaic materials is important so as to prevent large stresses and strains during fabrication and operation of the photovoltaic device. Here, we evaluate the structural, lattice dynamical, and thermodynamic properties of Ruddlesden-Popper chalcogenide Ba_{n+1}Zr_nS_{3n+1} (n=1,2,3, ∞) using the self-consistent quasi-harmonic approximation within density functional theory. These responses are compared to the thermal expansion of other Ruddlesden-Popper compounds and recent experimental data, which allows us to suggest guidelines for engineering thermal expansion in the Ruddlesden-Popper structure type with diverse chemistries. This work was supported by the National Science Foundation’s MRSEC program (DMR-1720139.) at the Materials Research Center of Northwestern University.

10:30 AM

(EMA-S6-011-2020) II-VI chalcogenide colloidal quantum dots for infrared applications (Invited)

P. Guyot-Sionnest*¹

1. University of Chicago, James Franck Institute, USA

Hg and Cd based chalcogenide colloidal quantum dot (CQD) have potential for infrared applications. A primary example is the zero-gap HgTe. Colloidal nanocrystals can be tuned across the infrared by adjusting the size from 4 to 15 nm. HgTe CQDs also exhibit decent photoluminescence, stable n or p doping, and good stability in ambient conditions. They have been used to fabricate photodetectors across the short-wave, mid-wave and long-wave infrared. With processing as a simple ink, these CQDs promise a vast reduction in cost and new fabrication paradigms compared with traditional HgCdTe single crystal wafer materials. This has been illustrated with dual band detectors, flexible detectors, detectors in Fabry-Perrot cavity and plasmon enhanced detectors. I will describe this progress and how this might transform infrared detection. The other chalcogenides, HgSe and SnSe, present also interesting properties. Notably, the low energy of the conduction band of both HgSe and zb HgS allows CQDs of these materials to be naturally n-doped, and exhibit intense intraband or plasmonic absorptions. CdS, CdSe and CdTe are lattice matched to their respective Hg chalcogenides, and core/shells or alloys will be significant as CQDs.

11:00 AM

(EMA-S6-012-2020) Order and disorder in nanosized oxides and chalcogenides (Invited)

V. Wood*¹

1. ETH Zurich, Switzerland

Nanoscale oxides and chalcogenides are useful in a wide range of devices including electrochemical energy storage and optoelectronics. In this talk, I will describe some of the challenges in characterizing these materials and approaches that can be used. I will describe two different studies. In the first, we consider the question: can vacancies exist stably in nanomaterials consisting of hundreds of atoms and can they order to form ordered vacancy compounds? Looking at the family of I-III-VI, we show that compositions known to form order vacancy compounds in the bulk can be achieved in the nanoscale and that ordering plays an important role in the electronic structure of these nanomaterials. We further show that the impact of disorder can be mitigated by introducing group II elements of intermediate valence. In a second study, we explore methods to examine the important role of interfaces in nanomaterials. Using LiFePO₄ as a model system, we show that by systematically synthesizing materials with controlled surface area to volume ratios, it is possible to use bulk techniques like inelastic neutron scattering to extract information on interface effects and surface treatments.

11:30 AM

(EMA-S6-013-2020) Pyroelectricity in semiconducting complex oxide

J. Shi*¹

1. Rensselaer Polytechnic Institute, USA

When crystals approach 2D, their ferroelectricity is destabilized or paraelectric-to-ferroelectric transition temperature decreases. How pyroelectricity scales with dimensionality remains largely unknown. In this talk, we attempt to answer this question with a complex oxide crystal as a model system. A Dion-Jacobson quasi-2D oxide down to a unit cell thickness is epitaxially grown on LaAlO₃ substrate by the molten salt-assisted liquid phase epitaxy following a screw-dislocation driven mechanism. We experimentally demonstrate switchable in-plane photo-ferroelectric and pyroelectric effects in our quasi-2D oxide. The observed size effect of pyroelectricity is explained by a few mechanisms such as electron-phonon renormalization and phonon anharmonicity.

11:45 AM

(EMA-S6-014-2020) A Semiconducting Quasi-2D Bismuth Oxide Perovskite

Z. Chen*¹; Y. Sun²; J. Shi¹

1. Rensselaer Polytechnic Institute, Materials science and engineering, USA
2. Shanghai Institute of Ceramics, China

In this work, we report the first experimental observation of ferroelectricity in a quasi-2D nanosheet Sillen-Aurivillius semiconducting split-ion oxyhalide perovskite with significant Rashba effect. Optoelectronic transport and temperature-dependent time-resolved photoluminescence studies show that layered perovskite crystal exhibits a direct band gap of 2.4 eV, considerable optical quantum efficiency and decent carrier dynamics, making it a promising candidate in photon-valley coupling. Electrical transport shows up to 100× current rectification in Bi₄NbO₈Cl single crystal nanosheet-based planar devices with symmetric graphite electrodes. By electrical poling, the diode polarity becomes switchable, yielding repeatable rectified current. Switchable rectification sustains in 13-unit-cell thick Bi₄NbO₈Cl nanosheet, and unswitchable rectification sustains even down to ~3-unit-cell limit. The in-plane ferroelectricity in the 2D oxide crystal leads to the observation of entropic pyroelectric behavior and a Rashba-type spin texture. The integration of appropriate bandgap, considerable visible light optical quantum efficiency, strong polarization and the strong Rashba-Dresselhaus spin polarization in one material provides a novel design paradigm for realizing emergent spin-orbitronics.

12:00 PM

(EMA-S6-015-2020) Free-Standing 2D Oxide Nanomaterials with Exotic Physical Properties (Invited)

X. Wang*¹

1. University of Wisconsin-Madison, Materials Science and Engineering, USA

Two-dimensional (2D) nanomaterials so far are primarily limited to naturally layered materials, i.e. van der Waals solids. Here, we demonstrate that surfactant monolayers could serve as a soft template supporting the nucleation and growth of 2D nanomaterials in large area beyond the limitation of van der Waals solids. This technique was denoted as Ionic Layer Epitaxy (ILE), through which 1 to 2 nm thick, single-crystalline free-standing ZnO nanosheets with sizes up to tens of microns were synthesized at the water-air interface. Mimicking the biomineralization processing by using mix charge surfactants led a successful synthesis of single-crystalline nanosheets from a broad range of functional oxide materials, including CoO, MnO₂, Bi₂O₃, etc. New physical properties emerged from the ultrathin geometry. For example, stable p-type conductivity was observed from the ZnO nanosheets as a result of electron depletion. High concentration of cation or oxygen vacancies could be controlled by the surfactant modulation, leading to superior

magnetic property and memristive behavior. Substantially enhanced electrochemical catalytic performance was also discovered from multiple ultrathin oxide systems. In general, ILE vastly broadens the range of 2D nanomaterials from layered van der Waals solids to oxide ceramics, opening up opportunities for discoveries of exciting transport, magnetic, photonic, and catalytic properties.

Advanced Characterization of Physical and Chemical Properties

Room: Magnolia A

Session Chairs: Andriy Zakutayev, National Renewable Energy Laboratory; Sage Bauers, National Renewable Energy Laboratory

2:00 PM

(EMA-S6-016-2020) Replica bands in FeSe monolayer on SrTiO₃ superconductors (Invited)

K. Zou*¹

1. University of British Columbia, Physics & Astronomy, Canada

The observation of replica bands in monolayer (ML) FeSe on SrTiO₃ (STO) superconductors in angle-resolved photoemission spectroscopy (ARPES) [1] has triggered intense discussions on the role of STO phonon coupling on its enhanced superconductivity. F. Li and G. A. Sawatzky [2] recently proposed an extrinsic photoelectron energy loss (PEL) mechanism for the replica bands, different from the intrinsic forward-scattering electron-phonon coupling proposed by J. Lee et al [1]. In the PEL process, the loss probability is proportional to the interaction time of escaping photoelectrons, leading to a strong photon energy dependence in the ratio of replica and main band. To date, the origin of replica band remains elusive as well as the mechanisms of the enhanced superconductivity in ML FeSe. We have conducted ARPES experiments using a wide range of photon energy to clarify the replica band origin. Our recent progress on different ML FeSe/oxides interfaces where the substrate has different phonon energies will also be presented.

2:30 PM

(EMA-S6-017-2020) Controlling light-matter interactions in chalcogenide-based topological semimetals: Novel physics to devices (Invited)

R. Agarwal*¹

1. University of Pennsylvania, Materials Science & Engineering, USA

Can one control photoresponse in materials via patterning optical fields? In this talk, we explore this idea on Weyl semimetals (WSMs), which are a family of gapless topological materials with broken inversion and/or time reversal symmetry. We will introduce a new nonlinear optoelectronic probe, which we call spatially dispersive circular photogalvanic effect (s-CPGE) and demonstrate its sensitivity to detailed band features owing to its unique excitation mechanism. In WSMs such as MoTe₂ and Mo_{1-x}W_xTe₂ in the inversion symmetry broken phase, we observe circulating photocurrent when illuminated with circularly polarized light at normal incidence. We will explain these observations from a new microscopic nonlinear response function theory by taking into account the optical field gradients. Our analysis shows that s-CPGE is controlled by a unique symmetry selection rule combined with asymmetric carrier excitation and relaxation dynamics. Recent results of s-CPGE performed over a wide spectral range shows the effect of band inversion and asymmetric electron relaxation effects on the response, from where important materials properties are extracted. These results also provide a new approach to controlling photoresponse by patterning optical fields on WSMs. The implication of our results to assemble chiral photodetectors for quantum photonic applications will be discussed.

3:00 PM

(EMA-S6-018-2020) Atomic Scale Elemental Analysis of Complex Oxide Thin Films and Heterostructures (Invited)J. Ravichandran*¹

1. University of Southern California, Chemical Engineering and Materials Science, USA

Complex oxides are a class of materials with broad diversity in the structural, chemical and physical characteristics. Pulsed laser deposition (PLD) of complex oxide films has unearthed several of these interesting phenomena and is slowly evolving into a commercially viable technique. The development of high pressure reflection high energy electron diffraction (RHEED) has revolutionized in situ structural characterization during PLD and unleashed atomic scale engineering of oxide heterostructures. In this talk, I will discuss my group's efforts in implementing an in situ and real time Auger electron spectroscopy to study chemical composition during pulsed laser deposition. We have used this method to sense several elements (>25) with monolayer level surface sensitivity. I will also discuss the use of this technique with RHEED to elucidate the dynamics of growth during PLD. I will also discuss our efforts in using ex situ elemental analysis methods such as neutron spectroscopy and secondary ion mass spectroscopy to understand the origin of the unexpected physical properties to the changes in their chemical composition. I will provide the future outlook for heterostructure engineering and advanced elemental and chemical analysis methods to discover and understand interesting physical phenomena in complex oxides.

3:30 PM

(EMA-S6-019-2020) A new family of anisotropic zinc-based semiconductors in a shallow energy landscape (Invited)A. Bhutani¹; X. Zhang¹; P. Behera¹; R. Thiruvengadam¹; S. Murray¹; A. Schleife¹; D. Shoemaker*¹

1. University of Illinois, USA

The grand challenge of synthesizing materials by predictive design remains outstanding because controlling all thermodynamic and kinetic factors that influence synthesizability quickly becomes intractable, even for well-known systems. Nevertheless, predictions that are strengthened by large amounts of quality data should have well-defined rates of success. Here we present a family of previously undescribed zinc-based semiconductors with wide band gaps in four ternary systems Na--Zn--Se, Na--Zn--S, K--Zn--Se, and K--Zn--S. All new phases spring from known structure types and indicate the possibility of many such phases hiding in easily-accessible phase space. Bond energy calculations from DFT reproduce the experimental convex hull in this system extremely well. The new phases presented here feature electronic structures best described as anisotropic analogs of the parent binaries ZnS and ZnSe. Our BSE calculations show a strong influence of electron-hole interaction and optical local-field effects on the optical properties of these materials, as evidenced by our accurate optical spectra of the pseudo-1D structures. Large optical anisotropy in this group of materials highlights their potential for birefringent applications.

S7: Superconducting and Magnetic Materials: From Basic Science to Applications**2D Correlated Materials I**

Room: Cypress B

Session Chair: Michael Osofsky, Naval Research Laboratory

8:00 AM

(EMA-S7-010-2020) The magnetism of double perovskites containing 5d transition metal ions (Invited)P. Woodward*¹

1. Ohio State University, Chemistry and Biochemistry, USA

In this talk I will discuss the magnetism of oxides containing 5d transition metal ions, which differ from their 3d transition metal oxide counterparts in several fundamental ways: (1) the 5d orbitals extend further from the nucleus which can lead to unexpectedly strong superexchange interactions, (2) for similar electron configurations the spin-orbit coupling of 5d ions is much stronger, and (3) competing magnetic ground states in 5d transition metal oxides are very sensitive to distortions of the lattice. In this talk I discuss our studies of the magnetic properties of $A_2MM'O_6$ double perovskites where M' is either osmium, rhenium, or iridium. I will discuss double perovskites where the 5d ion is the only magnetic ion in the structure, as well as double perovskites that contain both 3d and 5d ions. Ground states including antiferromagnetism, ferromagnetism, ferrimagnetism and spin glasses can be realized in this family of compounds. A common theme is an extreme sensitivity to changes in the filling of d-orbitals and/or distortions of the crystal structure.

8:30 AM

(EMA-S7-011-2020) Theory of the Quantum Spin Hall Effect in 2D Metals (Invited)A. Zhao¹; Q. Gu²; R. Klemm*¹

1. University of Central Florida, Dept. of Physics, USA

2. University of Science and Technology Beijing, Department of Physics, China

We propose an experiment to observe the quantum spin Hall effect in a two-dimensional (2D) metal that is qualitatively different from quantum spin Hall studies of 2D topological insulators. The center of a monolayer metallic annulus perpendicularly surrounds a long cylindrical solenoid containing magnetic flux Φ . Uniformly placed voltage leads along the inner and outer annular radii produce a potential difference Δv . The quantization of the azimuthal current can be measured by integral changes in both δ and $\delta \pm \gamma/2$, where $\delta = \Phi_s q/h$, $\gamma = q\Delta v/(mc^2) \ll 1$, h is Planck's constant, q is the charge of the conduction electron or hole, and mc^2 is its rest energy.

9:00 AM

(EMA-S7-012-2020) Stanene: A possible topological superconductor (Invited)J. Jia*¹

1. Shanghai Jiao Tong University, Physics and Astronomy, China

Stanene and its derivatives are predicted to be 2D topological insulators (TI) with a very large band gap as proposed by first-principles calculations, and support enhanced thermoelectric performance, topological superconductivity and the near-room-temperature quantum anomalous Hall (QAH) effect. Here, we report a successful fabrication of 2D stanene by MBE. The atomic and electronic structures determined by STM and ARPES agree well with the predictions by first-principles calculations. Bulk band gap and edge states are also observed. On stanene thicker than 2 layers, superconductivity is also observed, which suggests stanene is a good candidate for topological superconductor.

9:30 AM

(EMA-S7-013-2020) Interplay of Superconductivity, charge density wave and magnetism in layered 2D materials (Invited)

S. Li^{*1}; H. Wu²; S. Michael²; K. Taddei³; C. Dela Cruz³; T. J. Haugan⁴; B. Lv¹

1. University of Texas, Dallas, Dept. of Physics, USA
2. U.S. Air Force Research Laboratory, USA
3. Oak Ridge National Laboratory, USA
4. U.S. Air Force Research Laboratory, AFRL/RQOM, USA

The layered materials with weak van der Waals interlayer interaction have created a rich platform to exhibit exotic properties such as topology, magnetism, and superconductivity. In this talk, we will present several examples from our group demonstrating the interplay of superconductivity, charge density wave (CDW), and superconductivity in several layered 2D systems: 1) unusual superconductivity behavior in the chemical intercalated 1T semi-conducting SnSe₂ compound. CDW transition emerges together with the superconductivity in this system. Further intercalation with Co(Cp)₂, we observed the coexisting the superconductivity, CDW and ferromagnetism in this system. 2) Chemical intercalation studies of layered 1T' phase of TaTe₂ and NbTe₂ with CDW transition at 170K for TaTe₂ and above 550K for NbTe₂ respectively. And NbTe₂ show superconductivity below 0.74K. By intercalation of magnetic atoms, we are expecting to observe the interplay among superconductivity, CDW and magnetism in the NbTe₂ system. Indeed, through manipulation of the synthetic methods, we observed drastic changes of crystal symmetry and physical properties in the same material Fe_xNbTe₂ with ground state from spin glass insulator to canted antiferromagnetic metal. The details of these results will be presented and the rich interplay of superconductivity, CDW, and magnetism in these systems will be elaborated.

2D Correlated Materials II

Room: Cypress B

Session Chair: Jinfeng Jia, Shanghai Jiao Tong University

10:30 AM

(EMA-S7-014-2020) Superconductivity and Magnetic Ordering In 2D Materials and Heterostructures (Invited)

C. Lau^{*1}

1. The Ohio State University, Dept. of Physics, USA

Low dimensional materials constitute an exciting and unusually tunable platform for investigation of electronic, thermal, optical and mechanical properties that are often dramatically different from their bulk counterparts. Here I will present transport measurements of high quality few-layer two-dimensional materials. For instance, we have observed robust long distance spin transport through the antiferromagnetic state in monolayer graphene, superconductivity and insulating states in twisted bilayer graphene, and evidence for intrinsic magnetic ordering in few-layer graphene devices.

11:00 AM

(EMA-S7-015-2020) Effect of interface on the physical properties of superconductor nanocomposites and magnetic/insulator/magnetic heterostructures (Invited)

J. Wu^{*1}

1. University of Kansas, USA

In nanomaterials and devices, the role of the interface becomes increasingly important as the scale of materials approaches few to sub-nanometers. This talk highlights a few such examples including: 1) superconducting nanocomposites of one-dimensional insulating nanorods embedded in superconducting YBCO matrix; and 2) magnetic/insulator/magnetic (Fe/Al₂O₃ (2nm)/Fe) heterostructures. In the former, we have found the nanorod/YBCO interface of 1-2 nm in thickness plays a critical role in determining the magnetic vortex

pinning efficiency of the nanorods. A coherent nanorod/YBCO interface can yield pinning force density more than twice of the counterparts of semi-coherent interface. In the latter, the formation of a sub-nanometer FeOx interfacial layer at the Fe/Al₂O₃ interface leads to two capacitors, one is dielectric and the other, ferroelectric, connected in series, resulting in repeatable switch between positive and negative capacitance. These results illustrates the importance in understanding the physical and chemical properties of the interfaces in nanomaterials and nanodevices.

11:30 AM

(EMA-S7-016-2020) Transport spin polarization of Pt/ferromagnetic insulator bilayers (Invited)

M. Osofsky^{*1}; J. Prestigiacomo¹; P. Li²; Y. Suzuki²

1. Naval Research Laboratory, USA
2. Stanford University, Department of Applied Physics, USA

It has been shown that the anomalous Hall effect can be observed in platinum films deposited on a ferromagnetic insulator which implies the existence of a magnetic proximity effect. One of the key features of ferromagnetic metals is a net spin polarization of the carriers at the Fermi energy which enable the functionality of spintronic devices. In this presentation we show that spin polarized carriers are indeed present in Pt films of various thicknesses that were deposited on magnesium aluminum ferrite (MAFO) using point contact Andreev scattering. The results were obtained by extracting conductance vs. voltage data from I-V curves taken through contacts formed by driving a sharpened superconducting Nb tip into the Pt/MAFO samples. The resulting spectra were then analysed using a modified BTK theory of supercurrent conversion at a normal/superconductor interface to obtain the values of the transport spin polarization. The authors acknowledge the support of the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering under the Laboratory University Collaboration Initiative (LUCI) and Vannevar Bush Faculty Fellowship (funded by the Office of Naval Research through grant N00014-15-1-0045).

12:00 PM

(EMA-S7-017-2020) Ultrafast excitation of coherent magnons in 2D antiferromagnets (Invited)

X. Zhang^{*1}

1. University of Florida, Physics, USA

The recently discovered atomically-thin magnetic crystals provide a unique playground to develop new approaches to manipulate magnetism. Rapid progresses have been made that demonstrate the potentials of utilizing 2D magnets to construct novel spintronic devices. However, their spin dynamics, which are crucial for microscopic understanding and determine the fundamental limit of spin manipulation, still remain elusive due to the difficulty to characterize these micron-sized samples with conventional microwave techniques. In this talk, I will show how we can access and probe the collective spin-wave excitations in an antiferromagnetic bilayer CrI₃ with ultrafast pump-probe spectroscopy. Coherent oscillations are observed in the time-resolved spectra of magnetization, and are attributed to the magnon modes of antiferromagnetic resonance in bilayer CrI₃. Both the transverse and longitudinal magnon branches are identified, allowing us to extract magnetic anisotropy and exchange energies in these atomically-thin magnetic materials. In the end, I will demonstrate the great gate tunability of magnon frequencies, which is unique for the 2D magnetic system, and reveal the potential to control magnon landscape with flexible electronic devices.

Tailoring Properties of Superconducting and Magnetic Materials

Room: Cypress B

Session Chair: Timothy Haugan, U.S. Air Force Research Laboratory

2:00 PM

(EMA-S7-018-2020) Giant enhancement of critical current density at high field in superconducting (Li,Fe)OHFeSe films by Mn doping (Invited)

D. Li¹; J. Yuan¹; L. Yu¹; F. Zhou¹; K. Jin¹; X. Dong^{*1}; Z. Zhao¹

1. Institute of Physics, CAS, China

Mn-ion is successfully incorporated into nontoxic superconducting (Li,Fe)OHFeSe films. Remarkably, the critical current density is significantly enhanced from 0.03 to 0.32 MA/cm² under 33 T, and the vortex pinning force density monotonically increases up to 106 GN/m³, which is the highest record so far among all iron-based superconductors. Our results demonstrate that Mn incorporation is an effective method to optimize the performance of (Li,Fe)OHFeSe films, offering a promising candidate for high-field applications.

2:30 PM

(EMA-S7-019-2020) State-of-the-art Nb₃Sn Films by electrochemical Deposition (Invited)

E. Barzi^{*1}

1. Fermi National Accelerator Lab, USA

The Nb-Sn composite is obtained first by pulsed electrodeposition from aqueous solutions of Sn layers and Cu intermediate layers onto Nb substrates. The electroplating is performed at near room temperature and at atmospheric pressure. The Nb₃Sn superconducting phase is then formed through solid diffusion by reacting the multi-layered samples in inert atmosphere at a maximum temperature of 700°C. This technique was developed and made reproducible at FNAL in the last few years, and was already proven both on flat and cylindrical samples. One application for this method is for superconducting radiofrequency cavities (SRF) for accelerators, in which the internal surface of the Nb cavity is coated with Nb₃Sn. Since the thermal reaction to produce Nb₃Sn is performed at a maximum temperature of only 700°C, it is applicable also to SRF cavities made of Cu. Cu is preferred over Nb for the SRF cavity body for its excellent thermal properties and lower cost. This workshop is indeed a perfect opportunity to discuss other possible applications from fundamental electronics to electric aircraft.

3:00 PM

(EMA-S7-020-2020) Nano-size Magnetic Additions Contribution to YBa₂Cu₃O_{7-x} Flux Pinning

M. Sebastian^{*1}; N. Pierce⁴; I. Maartense³; G. Kozlowski²; T. J. Haugan³

1. UDRI, USA

2. Wright State University, Physics, USA

3. U.S. Air Force Research Laboratory, AFRL/RQQM, USA

4. Hohman Plating, USA

Research world-wide has focused on addition of many single and multi-phase inclusions of nanoparticles and nanorods to enhance flux pinning and improve critical currents (I_c s) of high temperature superconductor YBa₂Cu₃O_{7-x} (YBCO) coated conductors. Magnetic materials are interesting to consider as flux pinning additions because of their potential for very strong pinning strength by combining core pinning with pinning the magnetic flux of the vortices. This paper compares the study of different M magnetic phase additions to YBCO including M = BaFe₁₂O₁₉, La_{0.67}Ca_{0.33}MnO₃, SrRuO₃, and Y₃Fe₅O₁₂. Nanosize additions were incorporated by depositing multilayer (M/YBCO)_N films to minimize degradation of T_c , and varying volume % additions of M phase from 0.5 % to 5%. Results indicate that T_c onsets are depressed with magnetic additions, however in some cases interestingly without degrading

the transition width. With optimization of magnetic additions, a 50% increase of critical current density has been obtained for low magnetic fields of < 1T at 65K to 77K. Microstructural and superconducting properties will be summarized, including SEM & TEM analysis.

3:15 PM

(EMA-S7-021-2020) Raman Spectroscopy, Photocatalytic Degradation, and Stabilization of Atomically Thin Chromium Tri-iodide

D. L. Shcherbakov^{*1}; P. Stepanov¹; D. Weber¹; Y. Wang¹; J. Hu²; Y. Zhu²; K. Watanabe³; T. Taniguchi³; Z. Mao²; W. Windl⁴; J. Goldberger¹; M. Bockrath¹; C. Lau⁵

1. The Ohio State University, USA

2. Pennsylvania State University, USA

3. National Institute for Materials Science, Japan

4. The Ohio State University, Dept. of Materials Science and Engineering, USA

5. The Ohio State University, Dept. of Physics, USA

As a 2D ferromagnetic semiconductor with magnetic ordering, atomically thin chromium tri-iodide is the latest addition to the family of two-dimensional (2D) materials. However, realistic exploration of CrI₃-based devices and heterostructures is challenging due to its extreme instability under ambient conditions. Here, we present Raman characterization of CrI₃ and demonstrate that the main degradation pathway of CrI₃ is the photocatalytic substitution of iodine by water. While simple encapsulation by Al₂O₃, PMMA, and hexagonal BN (hBN) only leads to modest reduction in degradation rate, minimizing light exposure markedly improves stability, and CrI₃ sheets sandwiched between hBN layers are air-stable for >10 days. We will discuss implication of such knowledge for ultrathin electronic devices. By monitoring the transfer characteristics of the CrI₃/graphene heterostructure over the course of degradation, we show that the aquachromium solution hole-dopes graphene.

Application of Superconducting Materials

Room: Cypress B

Session Chair: Emanuela Barzi, Fermi National Accelerator Lab

3:30 PM

(EMA-S7-022-2020) Update on Aircraft Electric Propulsion, and Impact of Superconducting and Cryogenic Technology (Invited)

T. J. Haugan^{*1}

1. U.S. Air Force Research Laboratory, AFRL/RQQM, USA

The development of electric propulsion has progressed rapidly in the last 5-10 years, and is being promoted by the chief technology officer (CTO) of every major international aerospace company. The incentives for development are to begin address the problem of global CO₂ emissions, and to enable benefits including 2-5x higher energy efficiency, > 10x lower operation costs, and the potential to open up huge new markets utilizing small regional airports and hubs. There are now over 100 publically known companies working in the field, and many more private. The field is recently working on developing many technology pieces, including electric drivetrains, energy storage, and novel aircraft designs such as distributed propulsion. Another significant issue to address is the difficult problem of thermal management of waste heat from electric components. So-called 'conventional' technologies are understood to have fundamental limitations for specific power density, and efficiencies. This paper will summarize recent progress in this field, and also present on how superconducting/cryogenic technologies can overcome fundamental limitations of 'conventional' technologies for energy efficiency and power density. Acknowledgments: The Air Force Office of Scientific Research (AFOSR) and LRIR #18RQCOR100, and the U.S. Air Force Research Laboratory Aerospace Systems Directorate (AFRL/RQ)

4:00 PM

(EMA-S7-023-2020) Material Selection, Structures, and Processing for the Safe Operation of Very High Magnetic Field Superconducting Accelerator Magnets (Invited)

C. J. Kovacs^{*1}; M. D. Sumption¹; E. Barzi¹; E. W. Collings¹; M. Majoros¹; A. Zlobin²; D. Turrioni²

1. The Ohio State University, Materials Science and Engineering, USA
2. Fermi National Accelerator Laboratory, APS-TD, USA

The High Energy Physics community is seeking solutions to develop very high field superconducting accelerator magnets for the next series of upgrades for large discovery science facilities. Two composite material properties, stability and protectability, will be the focus of this talk. Research at The Ohio State University and Fermi National Accelerator Laboratory into developing higher stability and protectability superconducting cable-insulation composites will be described. The success of higher stability and protectability high temperature and low temperature superconducting composites is a necessity for next generation superconducting accelerator magnets.

4:30 PM

(EMA-S7-024-2020) Temperature dependence of specific heat capacity, thermal conductivity, and electrical resistivity of Fe-Co alloys (Invited)

G. Kozłowski^{*1}; M. Susner²; M. Farfel³; J. Horwath²; Z. Turgut²

1. Wright State University, Physics, USA
2. AFRL, Wright-Patterson AFB, USA
3. Materials Science and Engineering, Carnegie Mellon University, USA

Specific heat capacity (C), thermal conductivity, and electrical resistivity of four commercially available Fe-Co alloys in a temperature range between 3 K and 400 K have been studied. Various contributions to specific heat capacity from electron, phonon, magnon, and other mechanisms are investigated. Fundamental physical properties such as Debye temperatures, density of states at Fermi level, and lower temperature anomalies as a function of impurities and lattice imperfections are discussed. With increasing amount of impurities and lattice imperfections in these Fe-Co alloys, specific heat capacity measurements show a decrease in Debye temperature, effective exchange interaction, spin wave stiffness constant, Curie temperature, and temperature value T_{\min} at C/T minimum at very low temperature region (less than 10 K). In the same time, an increase in C/T value at its minimum and in an overall value of specific heat capacity has been observed. Scattering mechanisms that govern temperature dependence of thermal conductivity were inferred from Wiedemann-Franz law while Matthiessen approximation was used for interpretation of the temperature dependent electrical resistivity.

S9: Ion Conducting Ceramics

Fundamental Processes and Characterizations in Ion Conducting Ceramics for Energy Storage

Room: Citrus A

Session Chair: Jiamian Hu, University of Wisconsin-Madison

8:30 AM

(EMA-S9-009-2020) Study the Formation of Solid/Solid Interface using Synchrotron Probes (Invited)

Z. Chen^{*1}

1. Argonne National Lab, USA

Lithium ion batteries have been considered most promising technology for large scale applications like electrified vehicles and stationary energy storage. However, the combustible and highly volatile carbonates have been long blamed for intrinsic safety concern of lithium-ion batteries. Hence, all solid state lithium

battery has been considered a safer chemistry than the conventional lithium-ion chemistries. In order to achieve the goal of liquid-free, it is important to create a strong and stable solid/solid interface between the cathode materials and the solid state electrolyte. In this work, co-sintering is explored as a promising low cost approach for creating the functional solid/solid interface. Both high-energy X-ray diffraction and transmission X-ray microscopy were deployed to investigate the interaction of cathode material and the electrolyte during the co-sintering process.

9:00 AM

(EMA-S9-010-2020) Tuning oxygen diffusion kinetics and pathways in oxygen vacancy ordered heterostructures (Invited)

Y. Du^{*1}

1. Pacific Northwest National Laboratory, USA

Structurally ordered oxides exhibit a broad range of structural, compositional, and functional properties. As such, they have found widespread application in energy storage and conversion devices, particularly for use as electrocatalysts, cathodes, and solid state ionics. However, as-designed materials can undergo dramatic changes due to ion diffusion, which, in many cases, leads to performance degradation and device failure. This talk will highlight our most recent effort aiming to modify complex oxides through heteroepitaxy to achieve tunable functional properties. Combining in situ and environmental transmission electron microscopy (TEM), $^{18}\text{O}_2$ labeled time-of-flight secondary ion mass spectrometry (ToF-SIMS), and ab initio simulations, we elucidate the structural and chemical evolution pathways in selected materials systems and reveal how such changes impact their functional properties. Using Brownmillerite (BM)-structured $\text{SrFeO}_{2.5}$ (BM-SFO), a perovskite (ABO_3)-associated structure that contain ordered oxygen vacancy channels, as an example, we show that at relatively low temperatures, a topotactic phase transition between BM-SFO and perovskite SrFeO_3 (SrCrO_3) can be promoted, delayed, or prohibited based on the interfacial strain conditions, highlighting the importance of interface engineering in designing robust and efficient ion conducting materials.

9:30 AM

(EMA-S9-011-2020) Magnesium Diffusion in Fe_3O_4 films Grown on MgO (001)

L. Wangoh^{*1}; Z. Yang¹; L. Wang²; T. Kaspar³; S. Heald⁴; H. Zhou⁴; Z. Zhang⁴; V. Murugesan¹; Y. Du²

1. Pacific Northwest National Laboratory, EMSL, USA
2. Pacific Northwest National Laboratory, USA
3. Pacific Northwest National Laboratory, Physical and Computational Sciences Directorate, USA
4. Argonne National Laboratory, USA

Fundamental ion diffusion and ion diffusion induced phase transition processes govern the performance of many energy materials and energy storage devices. Epitaxial heterostructures with well-defined interfaces can be ideal model systems for such studies. In this work, we have investigated the evolution of structural and electronic properties of epitaxial Fe_3O_4 thin films grown by Molecular Beam Epitaxy on MgO (001) as a function of annealing conditions. The films were characterized in-situ by Reflection High Energy Electron Diffraction (RHEED) and X-ray photoemission spectroscopy (XPS) as well as ex-situ by scanning transmission electron microscopy/electron energy loss spectroscopy (STEM/EELS), X-ray Diffraction and Absorption spectroscopy. We show that Mg out-diffusion from MgO to Fe_3O_4 leads to a spinel $\text{Mg}_{1-x}\text{Fe}_{2+x}\text{O}_4$ structure with a Rocksalt $\text{Mg}_y\text{Fe}_{1-y}\text{O}$ interface layer. In particular, STEM imaging reveals that the fast Mg diffusion channels are correlated with antiphase boundaries and structurally ordered regions.

9:45 AM

(EMA-S9-012-2020) Alkali ion transport in layered MnO₂ and its 2-D mesostructured analogs: Operando study of ion intercalationS. T. Mixture^{*1}; M. Flint¹; P. C. Metz¹; A. Ladonis¹

1. Alfred University, MSE, USA

MnO₂ nanosheet assemblies can be synthesized by re-stacking MnO₂ sheets to form new layered crystals or as high porosity solids with crumpled sheets. We show that operando structural characterization tools shed new light on the intercalation mechanisms while also probing the atomic-scale defects and chemomechanical responses during charging, primarily of interest in pseudocapacitors. An operando measurement cell was developed for X-ray diffraction, PDF and XAS studies, which enabled accurate quantification of the interatomic spacings and defect content vs. charge state. The data demonstrate that the nanosheets breathe in 2-D; in other words, the interlayer spacing between nanosheets remains invariant while the nanosheets expand and contract in the plane of the sheet by as much as 1% during charging – but only when the sheets are poorly re-stacked. In the case of more crystalline restacking, the interlayer distance also responds during the charge and discharge cycles, though ultimately the in-plane response triggers charge transfer. Electrochemical kinetics support the differentiation between interlayer and surface ion transport. We suggest that these observations can be used to develop and optimize mesostructures for future supercapacitor, sensor and catalytic applications, especially for materials that suffer from degradation caused by chemomechanical strains.

10:30 AM

(EMA-S9-005-2020) Phase-Field Modeling of Mesoscopic Ion Conduction in Solid Electrolytes (Invited)J. Hu^{*1}

1. University of Wisconsin-Madison, Materials Science and Engineering, USA

Phase-field modeling is one of the most powerful mesoscale modeling tools for understanding and predicting the evolution of microstructure under external physical stimuli (e.g., thermal, mechanical, magnetic, electric, optical) as well as the responses (both global and local) of the materials to these stimuli. In this talk, an overview of existing works on the application of phase-field to solid electrolytes (for both solid oxide fuel cells (SOFCs) and solid-state batteries) will be given. The rest of the talk will be focused on our previous and recent works on phase-field modeling of ion transport in the three-phase composites of (La,Sr)MnO₃(electrode)/YSZ(electrolyte)/air in SOFCs as well as the Li-ion transport in nanoporous Li-S solid electrolytes and polymer/ceramic composite solid electrolytes. The talk will end with a brief summary on what phase-field modeling might be able to offer in terms of modeling the ion conduction as well as other transport behaviors in solid-state materials.

Emerging Ion Conducting Ceramics: Oxide and Halide

Room: Citrus A

Session Chair: Zhenxing Feng, Oregon State University

11:00 AM

(EMA-S9-014-2020) Defect-driven Metal Oxide Electrodes for Metal Ion Batteries (Invited)H. Xiong^{*1}

1. Boise State University, Materials Science and Engineering, USA

Metal oxide electrodes could provide a safer battery while maintaining high reversible capacity for rechargeable metal ion batteries. In recent years evidence has shown that transition metal oxides which have structural defects (e.g., vacancies and interstitials) at

cation sites with local disorder have the potential to offer higher capacity and better stability compared to ordered oxides. In this talk, we report our integrated experimental and computational study of a nanostructured amorphous niobium oxide (Nb₂O₅) electrode grown by electrochemical anodization for lithium ion battery. An irreversible phase transformation from amorphous to crystalline phase in Nb₂O₅ electrode is observed during the first discharging process. A new niobium oxide phase is formed which is driven by in operando electrochemically cycling with Li⁺. The newly formed niobium oxide electrode exhibits high capacity, superb rate capability and good cycle life. The electrochemical charge storage mechanisms of the new electrode will be discussed. Later in the talk, we will also discuss our recent work on engineering interfaces of metal oxide composite electrode for sodium ion batteries.

11:30 AM

(EMA-S9-015-2020) Soft Processing of Halide Perovskite Thin Films (Invited)Y. Zhou^{*1}

1. Brown University, School of Engineering, USA

Halide perovskites (HPs) have recently emerged as a new type of inorganic-based semiconductors, which have already transformed the photovoltaic field and been demonstrating their impacts on the broad electronics field. These materials are formed primarily with ionic and secondary bonds, which are in contrast with the covalently-bonded conventional inorganic semiconductors, and thus, they fall into the emerging class of inorganic-based soft semiconductors. Our studies have shown that ions in these HPs are unusually active upon external environmental conditions. Such characteristic has enabled us to invent ultra-soft chemical methods for processing HP thin films with tailored microstructures and properties. Fundamental mechanisms on the HP thin film formation will further be elaborated. The demonstrated processing sciences are expected to have lasting impacts on the general development of HPs based electronics and iontronics, which will be discussed as a perspective in this talk.

S11: New Directions in Sintering and Microstructure Control for Electronic Applications**New Directions in Sintering and Microstructure Control**

Room: Magnolia B/C

Session Chairs: John Blendell, Purdue University; Wolfgang Rheinheimer, Purdue University; Lauren Hughes, Lawrence Berkeley National Laboratory

8:30 AM

(EMA-S11-001-2020) In situ grain growth measurements reveal that grain boundary motion is anisotropic (Invited)G. Rohrer^{*1}

1. Carnegie Mellon University, USA

Near field High Energy X-ray Diffraction Microscopy, a non-destructive, synchrotron based 3D characterization technique was used to track the microstructural evolution of high purity polycrystalline Nickel annealed at 800°C. We tracked approximately 2000 grains over the six anneal states with grain orientation and spatial location as criteria for grain-to-grain mapping. It was observed that neither the size of a grain nor the number of its nearest neighbors are strongly correlated to a grain's volume change over the time scale of this experiment. However, a grain's environment was influential in determining whether a grain grows or shrinks. When the motion of individual grain faces was examined, strong correlations between

the orientation of the grain face in the crystal reference frame and its area change during annealing were observed. Grain faces with (111) orientations experienced the greatest changes in area and also increased in relative area.

9:00 AM

(EMA-S11-002-2020) Isolating Thermodynamic and Kinetic Contributions to Sintering of Zirconia using Model 2-Particle Experiments Incorporating Load Control (Invited)

S. J. Dillon*¹

1. University of Illinois Urbana-Champaign, USA

A variety of novel sintering processes have emerged in recent decades that enable sintering at lower temperatures, sintering to higher densities, and the production of novel microstructures and nanostructures. The geometric complexity of the sintering process, multiple competing capillarity driven processes, and the coupling of thermodynamics and kinetics in rate equations all create challenges for understanding the sintering process at a fundamental level. This is especially true when trying to understand the influence of an additional variable, such as applied field or environmental effects. This talk describes a new approach to directly measuring the grain boundary and surface diffusivities and energies using a model 2-particle sintering experiments performed at the microscale under load control during in situ transmission electron microscopy imaging. The approach is applied to characterizing sintering of cubic ZrO₂ and the results provide insights into the nature of defects controlling the sintering process. We envision that the approach provides an excellent basis for systematically studying more complicated sintering phenomena, and future opportunities will be discussed.

9:30 AM

(EMA-S11-003-2020) Solute-Drag versus Solute-Acceleration in Controlling Grain Growth of Alumina (Invited)

R. Moshe¹; R. Marder¹; P. Ghosh¹; L. Rudnik¹; W. D. Kaplan*¹

1. Technion - Israel Institute of Technology, Dept. of Materials Science and Engineering, Israel

Solute-drag is a known phenomenon where atoms in solution which segregate to grain boundaries (GBs) reduce GB mobility. A paradigm in ceramics is the case of MgO segregation to GBs in alumina, driven by the reduction of GB energy, and resulting in a refined microstructure during sintering or annealing. Doping alumina with CaO and/or SiO₂ is thought to form a glass phase at GBs, resulting in exaggerated grain growth at high temperatures. This work experimentally demonstrates that at Ca concentrations below the high temperature solubility limit, i.e. before secondary phase formation, Ca segregation accelerates GB mobility. The increased mobility due to Ca segregation is believed to be due to an increase in vacancy concentration in the immediate vicinity of the grain boundaries. Co-doping with Mg and Ca leads to a higher Mg solubility limit, and thus more Mg at the grain boundaries in balance with Mg in solution, and thus a reduced grain boundary mobility. Presumably grain boundary motion in alumina is via the motion of disconnections, which has been experimentally demonstrated for SrTiO₃. How dopants, including carbon, interact with disconnections will be discussed.

10:30 AM

(EMA-S11-004-2020) Flash Sintering and Electric Field Effects on Microstructural Evolution in ZnO Based Model Systems (Invited)

J. Nie¹; C. Hu¹; J. Luo*¹

1. University of California, San Diego, USA

This talk will first discuss a series of studies of flash sintering using ZnO as a model system [see a Viewpoint: Scripta 146: 260 (2018)]. First, a thermal runaway model has been developed to forecast the onset flash temperatures [Acta 94:87 (2015)]. Second, we showed

that ultrafast heating enables the rapid densification [Acta 125:465 (2017)]. Third, new technological innovations include (a) two-step flash sintering (TSFS) to densify ceramics with suppressed grain growth [Scripta 141:6 (2017)] and (b) water-assisted flash sintering (WAFS) that can flash a ZnO green specimen at room temperature to subsequently achieve >98% density in seconds [Scripta 142:79 (2018)]. Furthermore, the effects of bulk phase and grain boundary complexion transformations on the flash sintering of Bi₂O₃-doped ZnO will be presented [Zhang et al., Acta, under review (a preprint: SSRN 3365842)]. Beyond flash sintering, we will discuss our most recent observations of the electric field induced enhanced and abnormal grain growth in dense Bi₂O₃-doped ZnO specimens. Here, our ongoing studies use coupled aberration-corrected HAADF STEM characterization and large-scale DFT modeling to reveal an underlying grain boundary structural or complexion transition to be the root cause of the observed asymmetric grain growth under the applied electric current/field, including the occurrence of abnormal grain growth.

11:00 AM

(EMA-S11-005-2020) Current rate controlled flash sintering of Gadolinium doped ceria for tailoring the microstructure (Invited)

T. Prasad Mishra¹; R. Ingraci Neto²; R. Raj²; O. Guillon¹; M. Bram*¹

1. Forschungszentrum Juelich, IEK-1, Germany
2. University of Colorado, Dept. of Mechanical Engineering, USA

Flash sintering of oxide ceramics attracts increasing interest in the sintering community. Mostly, flash sintering is done in the voltage-to-current control mode, which enables densification of the ceramic within few seconds. Due to being out of equilibrium state, control of densification and grain growth of the specimen remains challenging. Recently current rate controlled flash sintering has shown to be a novel mode of flash sintering. In this mode, the current is applied from the beginning and raised at a constant rate to a predefined maximum current density. By controlling the current rate, the densification of the specimen can be controlled. Proof of concept was done using 10 mol. % Gadolinium doped ceria (GDC10) powder as starting material. Dog bone shaped samples were placed in a tube furnace heated to 680°C before applying the current. Then the current rate was varied between 20 mA min⁻¹ and 1000 mA min⁻¹ until the maximum current density of 200 mA mm⁻² was reached. The onset of flash was detected by the drop of electric field which was generated across the specimen. Microstructural investigations of the flash sintered samples revealed homogeneous grain size distribution along the gauge length. Remarkably, the microstructure of the flash sintered samples shows that the grain size could be tailored by adjusting the current rate.

11:15 AM

(EMA-S11-006-2020) Origin of high interfacial resistances in solid-state batteries

P. Xu¹; W. Rheinheimer*¹; S. Shuvo¹; L. Stanciu¹

1. Purdue University, School of Materials Engineering, USA

The large interfacial resistance between electrolyte and electrodes poses a significant roadblock for all-solid-state batteries. The formation of interfacial phases (interphases) has been identified as one of the most significant sources for such high resistance. Therefore, studying the mechanism of interphase formation, along with investigating its effect on ionic conductivity, could lead to the discovery of avenues towards designing high-performance all-solid-state batteries. In this work, we studied the interphase formation in the perovskite electrolyte Li_{0.33}La_{0.57}TiO₃ (LLTO) and spinel cathode LiMn₂O₄ (LMO) pair by co-sintering experiments via spark plasma sintering (SPS), as well as conventional sintering. At the LLTO/LMO interface, we observed both an interphase formed by interdiffusion, as well as a complexion-like amorphous layer. We directly characterized the complexion layer morphology by using HRTEM.

Analytical TEM and SEM were used to reveal the elemental composition of the interphase and the interdiffusion layer. Furthermore, we used impedance spectroscopy to measure the electrical properties of the LLTO/LMO interphase and identified the interfacial resistance from the interdiffusion induced interphase to be larger than the individual phases by a factor of 40, whereas the amorphous layer was not visible in the impedance.

11:30 AM

(EMA-S11-007-2020) Cold sintering of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

J. Cockburn²; R. Boston^{*1}

1. University of Sheffield, Materials Science and Engineering, United Kingdom
2. Knowles (UK), Hethel Engineering Centre, Chapman Way, Hethel, United Kingdom

Cold sintering offers new routes to access structure-property-function relationships in functional oxides. The low temperatures used restrict grain growth and can be used to retain particular morphologies or particle size in dense ceramics. Here we describe the use of cold sintering to create dense ceramics of the high temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) at 180 °C (versus usually 900-1000 °C). Water is used as the transient solvent which is perhaps surprising given the insolubility of YBCO, however we will show evidence that the cold sintering is driven by the well-known cracking effect experienced by YBCO upon exposure to water, followed by partial recrystallization at elevated temperatures. Another known property of YBCO is that it displays crystallographic alignment under applied pressure, which if retained in the final ceramic, can be exploited to improve critical current density. We show how the pressure applied during cold sintering orients the grains inside the ceramic, and that this is retained in the finished dense pieces. Using superconducting quantum interference device magnetometry, we demonstrate that the preferential alignment of grains can create enhanced critical current density in the ceramic, and show how this is dependent on the orientation of the ceramic pieces with respect to the applied magnetic field.

11:45 AM

(EMA-S11-008-2020) Cold Sintering Process for CeO_2

T. Zaengle^{*1}; A. Ndayishimiye²; S. Bang²; S. Berbanoa²; K. Tsuji²; S. T. Mixture¹; C. Randall²

1. Alfred University, Dept. of Materials Science and Engineering, USA
2. Pennsylvania State University, Dept. of Materials Science and Engineering, USA

We demonstrate successful cold sintering of cerium dioxide. CeO_2 was cold sintered at 300, 275, 250, and 200 °C under 103 MPa for 3 and 6 hours resulting in relative densities from 80 to 85%. The optimal conditions were found at 300 °C for 6 hours, but we note a chlorine impurity was present in the ceria powder. The resulting ceramic microstructures studied using scanning electron microscopy clearly retain nanoscale particles without exaggerated grain growth, with primary particle sizes remaining below 50nm. X-ray powder diffraction demonstrates that the crystallite size progressively increased from 10 to 29 nm with increasing temperature, accompanied by a slight reduction in crystallite microstrain. Electrical conductivity measured by two point AC impedance yielded an activation energy of 0.77eV for GDC over the temperature range of 350 to 650°C. Additional electrical property measurements will be reported for pure ceria and for gadolinium doped variants with density at or above 85%.

12:00 PM

(EMA-S11-009-2020) Microstructural Evolution of Cold Sintered Electroceramic Thick Films

R. A. Dorey^{*1}; E. Jakubczyk¹; U. Abubacar¹

1. University of Surrey, Mechanical Engineering Sciences, United Kingdom

Constrained sintering of ceramic films presents challenges due to reduced densification, interfacial reactions and substrate degradation. Cold sintering, combining mechanical pressure and moderate heating in the presence of water, has been shown to yield high density bulk ceramics as well as offering a route to overcome constrained sintering and material compatibility issue found in conventional sintering. Here we report on the microstructural evaluation and film-substrate interactions that occur during cold sintering of ZnO thick films on metallic and ceramic substrates. Cold sintering of films is dominated by particle reshaping in the absence of large-scale atomic migration. In this way the original particle size is broadly maintained while achieving a high density. The formation of a thick hydrated layer, via the reaction with water, is shown here to be an essential part of the process as it is this layer that facilitates matter redistribution. The method by which water is introduced is shown to be important from a manufacturing perspective with a need to ensure good penetration and consistent application. When combined with conventional sintering significantly higher levels of densification are observed with respect to films subjected to conventional sintering only due to the exceptionally high levels of intimate contact established between particles during the cold sintering process.

12:15 PM

(EMA-S11-010-2020) $\text{LaCr}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0.8$): A novel NTC ceramic for wide range of temperature sensing

Y. Wu¹; F. Guan^{*1}; X. Cheng²

1. Alfred University, Kazuo Inamori School of Engineering, New York State College of Ceramics, USA
2. University of Jinan, Shandong Provincial Key Lab. of Preparation and Measurement of Building Materials, China

$\text{LaCr}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0.8$) negative temperature coefficient (NTC) compositions were synthesized by conventional solid-state reaction and two-step sintering. XRD analysis revealed that the structure is a uniform solid solution of an orthorhombic perovskite phase LaCrO_3 , with Fe substituting for Cr. SEM images and calculated open porosity showed that the substitution of Fe for Cr resulted in a decrease in porosity. Higher density (~97% of theoretical) and smaller grain size (0.5-2 μm) compared to conventional sintering indicated that the two-step sintering methodology was a simple, effective and energy-saving strategy for ceramic densification. The effects of the Fe doping on the electrical properties were studied. As the Fe content increased, it was observed that the electrical resistivity ($\rho_{25^\circ\text{C}}$) firstly started to decrease, and then to increase within a wide range of 473.3-51505.3 $\Omega \bullet \text{cm}$, while the B value was kept in a narrow range from 3651 K to 4301 K. Such combination of $\rho_{25^\circ\text{C}}$ and B enabled these compositions to be used as potential candidates for NTC thermistors in a wide range of temperatures, spanning from -50°C to 300°C. X-ray photoelectron spectroscopy analysis confirmed the presence of Cr^{3+} , Cr^{4+} , Fe^{3+} and Fe^{4+} ions on lattice sites, which may have resulted from the hopping conduction. The novel NTC materials also demonstrate excellent stability.

S15: Functional Materials for Biological Applications

Synthesis, Functionalization, and Characterization of Biomaterials

Room: Citrus B

Session Chairs: Julia Glaum, Norwegian University of Science and Technology; Jennifer Andrew, University of Florida

8:30 AM

(EMA-S15-001-2020) Biocompatibility of piezo-particulate composites for tissue regeneration (Invited)

V. Jarkov¹; H. Khanbareh¹

1. University of Bath, Mechanical Engineering, United Kingdom

Electrical stimulation can promote cell regeneration, particularly in the case of organs with limited healing capability, such as the central nervous system (CNS). Piezoelectric scaffolds, that generate electrical surface charge upon a change in pressure, have the potential to be a paradigm shift in the field of neuroregenerative medicine by wireless interaction with cells to stimulate growth. In this work we show successful fabrication and characterisation of biocompatible potassium sodium lithium niobate (KLN) -polymer composites in the form of thin dense membranes and porous scaffolds. Firstly, composite scaffolds of cationised cellulose-KLN with varying KLN content are synthesised and characterised. These materials are shown to be non-cytotoxic and viable using a PC12 cells as a neuronal model. Furthermore AFM results show a clear increase in surface roughness as dispersion of particles increased, proving cell viability is independent of surface roughness after 24 hours. Secondly, structured polydimethylsiloxane (PDMS)-KLN composites are prepared via in-situ poling-dielectrophoresis to obtain high piezoelectric sensitivity while maintaining flexibility and their biocompatibility is investigated using subventricular zone Neural Stem Cells (NSCs). A high level of viability is observed after 4 days in culture.

9:00 AM

(EMA-S15-002-2020) Piezoelectric materials for autonomous, electric implants

J. Glaum^{*}; K. K. Poon¹; M. Zhuk¹; M. Rotan¹; M. Einarsrud¹

1. Norwegian University of Science and Technology, Materials Science, Norway

In recent years, the value of piezoelectric materials for biomedical applications has been unfolding. They can act as self-sustained suppliers of charge for tissue repair or as in vivo energy harvesting components. Biocompatibility and stable performance in the presence of body fluids determine a materials potential for the task. In some cases, it is necessary that living cells form a close interface with the implanted material and when hard- and/or soft-tissue integration of the implant material is desired, large, open pores allowing the ingrowth of cells and blood vessels, provide a clinical benefit. The potential areas of application for piezoelectric materials in the biomedical context are manifold, but for their transfer into clinical routines safe and reliable under the unusual biochemical boundary conditions of the body as well as the standardized pre-surgery handling routines has to be ensured. We have been investigating two piezoelectric ceramic systems – BaTiO₃ and (K,Na)NbO₃ - regarding their potential as functional implants with a focus on microstructural features, chemical stability within liquid environments and functional stability against a standardized sterilization routine. Even though both systems are of perovskite type, there exist distinct differences in their behavior, which will be discussed with respect to material chemistry, Curie temperature and electromechanical characteristics.

9:15 AM

(EMA-S15-003-2020) Tellurite-based glass, ceramics and optical waveguide developments for acoustic sensing in biological applications

J. Wang^{*}

1. NSYSU, Taiwan

Tellurite-based materials have many compromising properties among oxide, fluoride and chalcogenide materials. They are: a reasonably wide transmission region (0.35–5 μm), versus only 0.2–3 μm for silicate glasses, good glass stability, a relatively low phonon energy among oxide glass formers, and high refractive index and high nonlinear refractive index, which are generally low in both fluoride and silicate material. Furthermore, tellurite has high sensitivity of acousto-optics (AO). We first investigate crystalline tellurite, tellurite ceramics with doping, amorphous tellurite and their optical waveguides dependences on acoustic sensing for biological applications. In the early stage, the AO sensing focuses on heart beat monitoring for diagnostic applications. Comparing to traditional acoustic sensor (i.e. piezo type), the tellurite can potentially offer simultaneously monitoring various frequencies of heart beat and higher acquisition rate by optics means. In this case, hopefully many weaker and earlier stage diseases of heart can be diagnosed. Furthermore, both single-mode and multimode tellurite waveguides will be fabricated. Compared with conventional devices, their AO dependence on both acoustic frequency and acoustic intensity of heart beat will be presented. Potential diagnostic applications of early stage heart-beat diseases will also be discussed.

9:30 AM

(EMA-S15-004-2020) Piezoelectric Biomaterials and Biocompatible Ferroelectrics (Invited)

B. Rodriguez^{*}

1. University College Dublin, School of Physics, Ireland

Piezoelectric biomaterials are being considered for numerous sensing and nanoelectronics applications. At the same time, biomedical applications of inorganic piezo- and ferroelectric materials continue to grow. Progress in understanding and exploiting the piezoelectric properties and surface charge of these functional materials will be presented. Aligned collagen I films prepared with different fibril sizes have been investigated to explore whether the characteristic 'piezoelectric domain' size of the films can be controlled. Unlike collagen, domains of uniform polarization can be electrically-poled at a ferroelectric surface. Such charge-patterned surfaces could be used to elicit a particular cell response and may find application in surface modification of implants, microfluidic devices, etc. In this work, the biocompatibility of BiFeO₃ and lithium niobate (LN) – including photodeposited gold, silver, and bimetallic LN templates – was investigated. The biocompatibility of LN templates with gold nanoparticle arrays suggests opportunities for Raman-based cell sensing applications. To explore LN as a neural substrate, a microfluidic chip was bonded to LN surfaces patterned by etching to create isolated axon microenvironments with predefined topographical cues. Such in vitro devices could be used to understand how neurons integrate different stimuli.

10:30 AM

(EMA-S15-005-2020) Functionally-Designed Ceria Nanostructures for Cell Therapies and Drug Delivery (Invited)

P. Koshy^{*}; S. Mofarah¹; R. Mehmood¹; J. L. Yang²; C. C. Sorrell¹

1. UNSW, School of Materials Science and Engineering, Australia
2. UNSW Sydney, Lowy Cancer Centre, Australia

Ceria (CeO₂) is a functional material that is increasingly used in biomedical applications owing to its redox behavior which allows it to switch readily between its oxidation states (Ce³⁺/Ce⁴⁺) depending on the pH of the environment. This allows ceria to function either as a prooxidant or as an antioxidant for different cell therapies.

Ceria can be tailored to be highly defective (CeO_{2-x}). The defects in CeO_{2-x} are mostly created on the surface allow it to show superior properties for surface-related applications in catalysis and biosensing. Therefore, controlling the density of exposed surfaces plays a critical role in improving the functionality of ceria. Despite recent progress in fabricating ceria nanostructures, existing shortcomings with regard to bioadsorption, kinetics of dissociation, biocompatibility, and biocatalytic activity have limited their use for biomedical applications. Research by our team has successfully fabricated ceria nanostructures of varying dimensionality and high functionality using novel, cost-effective, controllable, chemical agent-free fabrication methods. Moreover, the work has developed novel functionalization approaches to overcome physiological issues such as protein adsorption and solubility issues in biological fluids while enhancing targeted delivery of nanoparticles to cells for cancer treatment and other cell therapies.

11:00 AM

(EMA-S15-006-2020) Materials for Phosphorus Recovery and Sustainability

J. L. Jones*¹; Y. Zhi²; D. Call²; D. Knappe²

1. North Carolina State University, Dept. of Materials Science & Engineering, USA
2. North Carolina State University, Civil, Construction, and Environmental Engineering, USA

Phosphorus (P) is a critical component of cellular structures like DNA and processes like energy transfer and underpins the productivity of food systems as a key nutrient in fertilizers. Yet many challenges exist around the availability, application, management, and disposal or reuse of P: P is sourced from non-renewable phosphate rock, is inefficiently utilized in agriculture, and can run off into surface waters causing algal blooms and hypoxia of marine life. Current technologies for removing environmental P are insufficient and have ill-defined impacts. For example, P can be scavenged from water with La-doped bentonite (Phoslock®) particles. Because this product settles to the bottom of water bodies, the long-term fate of P and La in the environment is unknown. New materials and processes are needed to more sustainably recover P from various water sources and enable P reuse in agriculture. Our work involves fundamental studies of processes such as adsorption/desorption, precipitation/dissolution, and intercalation of P-containing compounds and complexes in functional (nano)materials within complex environmental matrices, such as municipal wastewater and lake water. Initial materials under study included Phoslock®, $\text{La}_2(\text{CO}_3)_3$, MgO , and hematite. We will present our results of efficiency and effectiveness of P recovery from matrices as well as X-ray and electron characterization techniques to determine mechanisms.

11:15 AM

(EMA-S15-007-2020) Magnetolectric Nanomaterials and their Potential for Biomedical Applications

J. Andrew*¹

1. University of Florida, USA

Electric fields are ubiquitous throughout the body, playing important roles in a multitude of biological processes including angiogenesis, cell division, cell signaling, prenatal development, wound healing, and neural stimulation. An increased understanding of the role of electric fields in the body has led to the development of devices for biomedical applications that incorporate electromagnetic fields as an intrinsically novel functionality (e.g., bioactuators, biosensors, cardiac/neural electrodes, and tissues scaffolds). However, in the majority of the aforementioned devices an implanted power supply is necessary for operation, and therefore requires highly invasive procedures. Here, we report on the potential of magnetolectric-based composites to overcome this challenge. Magnetolectric materials are capable of producing localized electric fields in response to an applied magnetic field, which the body is

permeable to. Here, we present on the potential of magnetolectric materials to be utilized in biomedical applications, with a focus on neuronal stimulation for regeneration purposes. We will identify key challenges in this field, such as the synthesis and characterization of biocompatible magnetolectric materials, challenges in experimental design, and opportunities for future research that would lead to the realization of magnetolectric biomaterials and their applications.

11:30 AM

(EMA-S15-008-2020) A Global perspective of Nanoceria surface Chemistry: Steps towards predictive Nano-engineering (Invited)

S. Seal*¹; D. Sayle²; M. Molinari³

1. University of Central Florida, Mat. Sci. Eng, College of Medicine, USA
2. University of Kent, United Kingdom
3. University of Huddersfield, United Kingdom

Cerium oxide nanomaterials (nanoceria) have undergone extensive research with applications in widely varying biomedical applications (e.g. biomedical sensors, artificial enzymes/nanozymes). The biomedical activity/utility of these materials arises from the oxygen uptake/release behavior of defect surface sites and $\text{Ce}^{3+}/\text{Ce}^{4+}$ redox couple along with the formation/loss of oxygen vacancies. Many studies have attributed observed enzyme-mimetic (e.g. superoxide dismutase, catalase) redox activity to the relative concentrations of these redox states within nanocrystals. However, we have demonstrated, in several experimental and theoretical studies, the greater intricacy of these reactions. In particular, water adsorption favorability for varied crystal planes, atomic density of surface facets, density of terminal hydroxyl groups, and the presence of ledge-like [110] facets have been implicated in observed catalytic reactivity. Further, the influence of pH and of chemical environment (e.g. water, biological media and cells) have been investigated. Future studies of nanoceria will require a more comprehensive understanding of the complex inter-actions among these features for the synthesis of application-tailored, nano-engineered material formulations.

Therapeutic, Diagnostic, and Biosensing Applications

Room: Citrus B

Session Chairs: Julia Glaum, Norwegian University of Science and Technology; Hamideh Khanbareh, University of Bath

2:00 PM

(EMA-S15-009-2020) Piezoelectric Biomaterials for Tissue Regeneration (Invited)

T. L. Arinze*¹

1. New Jersey Institute of Technology, USA

Tissue engineering and regenerative medicine approaches for rebuilding damaged or diseased tissues have shown promise. Stem cells have been sought as an attractive cell source to be used in combination with biomaterials that act as scaffolds to regenerate tissues. Recent discoveries have shown that the properties of the scaffold can influence stem cell self-renewal and/or differentiation, which has had a tremendous impact on identifying strategies for using these cells effectively in the body. This presentation will describe studies examining the influence of biomaterials on stem cell behavior with an emphasis on recent results using piezoelectric polymers and composites that provide electromechanical cues to stem cells and other cell types. The electromechanical properties of these biomaterials can be tailored to promote the differentiation of stem cells along different lineages and promote tissue formation. These biomaterials and their potential use for neural and orthopaedic applications will be discussed.

2:30 PM

(EMA-S15-010-2020) Graphene Nanocomposite based Nano Materials Case Study: As an Electrochemical Biosensor

A. Nemati¹; N. Ahmadi²; M. Bagherzadeh⁴; E. Nemati³

1. Sharif University of Technology, Department of Materials Science & Engineering, Islamic Republic of Iran
2. Science and Research Branch, Islamic Azad University, Department of Materials Engineering, Islamic Republic of Iran
3. Ecole de Technologie Superieure, Mechanical Engineering, Canada
4. NSTRI, Material Research School, Islamic Republic of Iran

A class of nano materials based on graphene nanocomposites was synthesized to compare the effects of graphene and graphene QD on the photoelectric properties as a biosensor. The nanoparticles of titania, ceria, and cerium-doped titania as well as tania-ceria-graphene QD nanocomposite (using hydrothermal method) were synthesized and characterized (by different techniques), after calcining at different temperatures. Finally, the glassy carbon electrode surface was modified by optimal nanocomposites. Electrochemical and photo-electrochemical tests of dopamine biosensors were performed in the presence of dopamine interfering agents such as ascorbic acid and uric acid. According to the obtained results, the electrical conductivity of CedT/RGO nanocomposite was increased from 4.6 ($\mu\text{S}/\text{cm}$) to 81.3 ($\mu\text{S}/\text{cm}$). In addition, the absorption spectrum of the nanocomposite was shifted toward visible wavelengths. The band gap of the titania was reduced from ~ 3.2 eV to ~ 2.65 eV in CedT nanoparticles and it was further reduced to ~ 1.95 eV in the CedT/RGO nanocomposite. The results showed that Titania-Ceria-reduced Graphene oxide nanocomposite for dopamine electrochemical biosensor with a linear range from 1 μM to 500 μM . Meanwhile, with Graphene QD nanocomposite as an electrochemical biosensor for dopamine with a linear range of 0.3 μM to 750 μM were selected as optimal compounds.

2:45 PM

(EMA-S15-011-2020) Biodegradable Piezoelectric Polymers for Medical Applications (Invited)

T. D. Nguyen^{*1}

1. University of Connecticut, USA

Measuring vital physiological pressures is important for monitoring health status, preventing the buildup of dangerous internal forces in impaired organs, and enabling novel approaches of using mechanical stimulation for tissue regeneration. Pressure sensors are often required to be implanted and directly integrated with native soft biological systems. Therefore, the devices should be flexible and at the same time, biodegradable, to avoid invasive removal surgery that can damage directly-interfaced tissues. Despite recent achievements in biodegradable electronic devices, there is still a tremendous need to develop a force sensor which only relies on safe medical materials and requires no complex fabrication process to provide accurate information on important bio-physiological forces. Here, we present a new strategy for material processing, electromechanical analysis, device fabrication, and assessment of a new piezoelectric Poly-L-lactide (PLLA) polymer to create a biodegradable, biocompatible piezoelectric force-sensor which only employs medical materials used commonly in FDA-approved implants, for the monitoring of biological forces. The sensor can be integrated with tissues and organs, forming self-sensing bionic systems to enable many exciting applications in regenerative medicine, drug delivery, and medical devices.

Failure: The Greatest Teacher

Room: Orange B

Session Chair: Geoff Brenneka, Colorado School of Mines

5:00 PM

(EMA-FAIL-001-2020) Bulldozing through nanoscale mistakes (er... DISCOVERIES!) (Invited)

B. Huey^{*1}

1. University of Connecticut, Materials Science and Engineering, USA

Let's face it, anyone who has ever tried AFM recognizes that it involves as much art as it does science. No, I don't mean that we paint our results. But it is sufficiently complicated that it requires "10,000 hours" to master. Otherwise, mistakes can easily lead to misinterpretations: 'representative' observations may not actually be reproducible; surface features may mask the effects we really want to investigate; and the sharp and fragile tip will likely in fact be broken. Each of these can obfuscate the results for all but the most expert AFM users. In fact, these have been persistent challenges for the past >30 years since the invention of AFM, largely resulting from our community's principle rule: protect the probe! But we can sweep away most of these problems by literally sweeping clear the surface. Or as we fondly think of it in the Huey AFM Labs—bulldozing the sample (carefully...and of course at the nanoscale). After all, archeologists use a toothbrush to expose dinosaur bones. We'll show examples where we've done the same at UConn. Just with much smaller 'dinosaurs.'

5:30 PM

(EMA-FAIL-002-2020) Sintering - Science, Art or Luck? (Invited)

J. Blendell^{*1}

1. Purdue University, USA

Every student is taught that sintering is a well understood process that is driven by the reduction in surface area of the powder compact. In practice it never works out quite the way we teach it. The ability to produce materials with controlled density, grain size, and microstructure often involves a mixture of science, experience, and good fortune. In practice we find many systems that are unsinterable using simple compaction and heating. We then look to the suite of tool (aka tricks) that are known to aid sintering. The addition of MgO to Al_2O_3 was the first case of making something sinterable to full density. But finding a similar magic additive or even understanding the role of MgO has been elusive. The use of applied pressure, fast heating, unique temperature profiles, and electric fields have been successful in some cases and failures in others. In many systems even using all the tricks does not result in a useful sample. In this talk I will present a process for solving any sintering problem. This does not mean that you can sinter anything, but there are pathways you can follow to increase your chances. I will also present how we were unsuccessful in sintering the MgO-NiO system and how we solved the problem. It was not pretty but the student did graduate.

Author Index

* Denotes Presenter

A	
Abubacar, U.	75
Adamchuk, D.	22
Adhikary, G.	40
Afshari, E.*	28
Agarwal, R.*	68
Aggoune, W.	47
Ahmadi, N.	78
Aimi, A.*	39
Akhtar, M.	33
Akkopru Akgun, B.	17
Albe, K.	55
Albrecht, M.	47
Alff, L.	27
Allen, L. J.	9
Almonte, F.*	16
Alpay, P.	29, 32, 65
Amamou, W.	9
Amoroso, D.	21
Andrew, J.*	77
Andrews, S.	35
Arca, E.	32
Arinzeh, T. L.*	77
Artrith, N.*	30
Aryana, K.	38
Aryana, K.*	59
Asandei, A.	39
B	
Babakhani, A.*	28
Badding, M.	27
Bae, J.	36
Baek, D.	9
Bagherzadeh, M.	78
Bagues Salguero, N.	18
Baker, J.	20, 23, 24
Balachandran, P.*	48
Balakrishnan, G.	21
Balatsky, A.	32
Balciunas, S.	22
Balciunas, S.*	35
Balke Wisinger, N.	13
Balke Wisinger, N.*	63
Bang, S.	75
Banys, J.	35
Banys, J.*	22
Barnes, P.	38
Baros, A. E.	29, 43
Bartek, N.*	33
Bartel, C.	32
Barzi, E.	72
Barzi, E.*	71
Barzilay, M.	7, 66
Bauers, S.	32
Bauers, S.*	67
Bayard, H.	51
Bazarov, I.	61
Beaton, D.	13
Bedzyk, M.	40
Beechem, T. E.*	19
Beer, S.	64
Behera, P.	69
Belhadi, J.	14
Bell, A. J.	37
Bencan, A.	53
Benedek, N.	28
Berbanoa, S.	75
Berger, M.	54
Bernal, B.	38
Berweger, S.	58
Beyer, K.	37
Bhutani, A.	69
Biswas, B.	13
Blanchet, M.	37, 61
Blanchet, M.*	48
Blendell, J.	44
Blendell, J.*	78
Bobnar, V.	23
Bock, J. A.	53
Bockrath, M.	71
Bohr, C.	64
Bokov, A. A.	22
Bonnett, T.	56
Borchers, J.	47
Börger, J. M.*	24
Borkiewicz, O.	37
Borman, T. M.*	64
Boston, R.*	75
Bosworth, B.	28
Bouchenoire, L.	15
Bourdarot, F.	21
Bouton, W.	27
Bouyanfif, H.	14
Bowden, M.	18, 46
Bowers, W.	48
Bowes, P. C.	23, 24
Bowes, P. C.*	24
Bradlesko, A.	10, 53
Brahlek, M.	45, 48
Bram, M.*	74
Braun, J. L.	38
Bredar, A. C.	48
Brehm, J. A.	63
Brennecka, G. L.*	27
Brown-Shaklee, H. J.	37
Brown, H. G.*	9
Brumbach, M.	12, 16
Brummel, I. A.*	37
Buckner, H.	25
Burton, A.	37
Buscaglia, V.	21
C	
Cabral, M. J.	20, 53
Cain, M.	42
Caldwell, J.	19, 20
Call, D.	77
Campanini, M.	13
Cann, D.	11, 33, 41, 42, 52
Caño, I.	63
Canu, G.	21
Cao, C.	51
Carbone, G.	15
Carcan, B.	14
Castillo, M. E.	14
Ceder, G.	32
Celuch, M.*	58
Chae, S.	36
Chae, S.*	64
Chambers, S.	18, 46
Chang, Y.*	51
Char, K.	47
Che, S.	11
Chen, A.	14, 39, 45
Chen, A.*	17
Chen, H.	19, 51
Chen, L.	28, 51
Chen, R.	11, 12
Chen, T.	25
Chen, X.	20, 51
Chen, Z.	9
Chen, Z.*	68, 72
Cheng, H.	9
Cheng, X.	75
Cheng, Y.	53
Chikara, S.	48
Cho, J.	35
Choi, E.	45
Choi, W.	36, 46
Choi, W.*	17
Choi, Y.	45
Chopdekar, R.	16, 45
Choudhary, K.*	13, 50, 63
Chu, B.*	10
Chu, M.	36
Chueh, W.	8
Ciomaga-Hatnean, M.	21
Ciston, J.	9
Cleri, A.*	20
Co, K.	29, 65
Cockburn, J.	75
Coker, E.	53
Coll, M.*	63, 64
Collazo, R.	25, 65
Collings, E. W.	72
Collins, L.	13
Colsmann, A.*	62
Comes, R. B.	37, 48, 61
Comes, R. B.*	15
Conley, J. F.*	12
Constantin, C.	16
Creange, N.*	20
Cruickshank, D.	27
Cui, J.	10
Culbertson, C. M.	12, 41
Culbertson, C. M.*	33
D	
Dai, M.	15
Dames, C.	11
Damjanovic, D.	42, 53
Daneu, N.	23
Daniels, J.	36, 44
Davids, P.	12, 16
de Andrade Scalvi, L. V.	34
de Oliveira Machado, D. H.*	34
De Souza, R. A.	24, 26
Dela Cruz, C.	70
Deluca, M.	21
Deng, H.	8
Desautels, R.	45
Devi, A.	64
Devkota, J.	55
DiAntonio, C.	18
Dias da Silva, J. H.	34
Dickey, E. C.	20, 25, 26, 41
Dickey, E. C.*	40
Dietlein, M.	15
Dillon, S. J.*	74
Dittmann, R.*	55
Dixon, K. E.*	38
Dkhil, B.*	19
Dolgos, M.	22, 33, 37, 41, 42
Dolgos, M.*	12
Dong, X.*	71
Donovan, B. F.*	58
Dorey, R. A.*	75
Draxl, C.	47
Drazic, G.	53
Du, Y.	18, 72

Author Index

Du, Y.*	72	Galib, R.	38	Hennig, R. G.*	50
Dubey, A.*	14	Galib, R.*	38	Henry, M. D.	12, 16
Ducharme, S.	39	Ganesh, P.	13, 46, 63	Hermann, R.*	15
Dwaraknath, S.	13	Gao, R.	11	Heron, J.	15, 64
Dynys, F.	38, 43, 54	Gao, X.	19, 45, 46	Heron, J.*	64
E					
Eckstein, U.	52	Garcia, C.	57	Herring, P.	8
Einarsrud, M.	76	Garcia, D.	11	Hershkovitz, A.	7
El Baggari, I.*	9	Garten, L.*	13	Hilario, M.	29, 43
El Marssi, M.*	14	Gaskins, J.	38, 59	Hilario, M.*	34
Elangoval, H.	7, 66	Gehring, M.	43, 55	Hill, M. D.*	27
Ellison, C.*	57	Geprags, S.	15	Hill, R.	53
Engel-Herbert, R.	19, 66	Ghanekar, P.	31	Hire, A. C.*	51
Enright, L.*	29	Ghosez, P.	21	Hirschfeld, P. J.	50
Erb, K. C.	44	Ghosh, A.*	39, 60	Hirt, B. D.*	35
Erni, R.	13	Ghosh, P.	74	Hlinka, J.	23
Ertekin, E.	25	Gibbons, B.	11, 52	Hlinka, J.*	44
Esposito, V.	43	Gild, J.	38	Hoang, A.	43, 55
Esteves, G.	16	Ginley, D.	13	Hoff, B. W.	29, 43
Evans, P. G.*	15	Giri, A.*	58	Hoffmann, C.	8
F					
Fahrenholtz, W.	38	Glaum, J.*	76	Hoffmann, M. J.	62
Falmbigl, M.	66	Gliebe, K.*	36	Hoglund, E.	19, 59
Fan, M.	19	Goetzee-Barral, A.	37	Holder, A.	32
Fan, Z.	10	Goldberger, J.	71	Holston, T.	54
Fan, Z.*	55	Gomez, C.	35	Hopkins, P. E.	19, 20, 38, 58, 59
Fancher, C.	16	Gong, Y.	47	Hoque, M.*	38
Fancher, C.*	8	Gonzales, J.	29	Horwath, J.	72
Farfel, M.	72	Gopalan, V.	13	Hossain, M. D.	64
Farghadany, E.*	18	Gorman, B.	13, 27	Hosseini, S.*	59
Farmer, T.	45	Gorzkowski, E.	65, 66	Hou, D.	12
Farnum, B.	37, 48	Grabowski, C.*	27	Hovden, R.	9, 15, 64
Fattakhova-Rohlfing, D.*	31	Gradauskaite, E.*	13	Howe, J.	19, 59
Fecht, H.	34	Greaney, A.	59	Hu, C.	74
Feldman, A. D.	28	Greeley, J.	31	Hu, J.	15, 51, 71
Feng, Z.	33, 41, 54	Grigalaitis, R.	22	Hu, J.*	73
Feng, Z.*	54	Grobis, M.	59	Huanca, D. R.	39
Ferreira, P.*	8	Gross, M.	53	Huang, B.*	30
Ferri, K.	65	Gross, M.*	53	Huang, H.	25
Ferri, K.*	18	Gross, R.	15	Huang, J.	18
Fichthorn, K.*	62	Groszewicz, P.	21	Huang, Y.	66
Fiebig, M.	13	Grove, K. M.*	11	Huber, D.	7
Fields, S.	16	Grudt, R.*	43	Huddleston, W.*	38, 54
Fields, S.*	16	Gu, Q.	69	Huey, B.	16, 39, 62
Filipic, C.	21	Guan, F.*	75	Huey, B.*	66, 78
Findlay, S.	9	Guennou, M.*	21	Hughes, L. A.*	8
Finkel, P.	42	Guillon, O.	31, 74	Hwang, J.*	25
Finkel, P.*	22	Gulgun, M. A.*	7	Hwang, W.*	32
Firor, D.	27	Gupta, I.*	12	I	
Fix, T.*	63	Gupta, S. K.	11	Ihlefeld, J.	12, 16, 19, 37
Fleig, J.*	55	Guyot-Sionnest, P.*	67	Ihlefeld, J.*	16
Flint, M.	73	H			
Floyd, R.	18	Hagerstrom, A.	29	Ingraci Neto, R.	74
Fohtung, E.	45	Haile, S. M.*	40	Irving, D. L.	20, 24
Foley, B.	56	Hall, D. A.*	11	Irving, D. L.*	23
Folland, T.	19	Hamlin, J. J.	50	Isaac, B.	47
Fonseca, E. C.*	51	Hammouri, M.	45	Itasaka, H.	42
Fox, A.*	28	Han, M.	46	Ivanov, M.	35
Franco, A. A.*	61	Han, T.	32	Ivanova, M. E.*	31
Freeland, J.	45	Hancock, H.	27	Ivry, Y.*	7, 66
Freysoldt, C.	24, 32	Harrington, G.*	25	J	
Fromling, T.*	43, 55	Harris, V.	56	Jablonskas, D.	22
Fthenakis, Z.	22	Haskel, D.	45	Jakoby, R.	27
Fujimoto, K.	39	Haugan, T. J.	70, 71	Jakubczyk, E.	75
Funni, S.*	41	Haugan, T. J.*	71	Jalan, B.	61
G					
Gabor, U.	66	Haumont, R.	21	Jalan, B.*	49
Gabor, U.*	23	Hayden, J.	64	Jamali, B.	28
Galdi, A.	61	Hayden, J.*	16	Janolin, P.*	56
		Hayden, S. C.	43	Jarkov, V.	76
		Heald, S.	48, 72	Jason, L.	48
		Heinselmann, K.	32	Jaszewski, S. T.	16
		Hennig, R. G.	24, 31, 32, 51, 61, 62	Jeen, H.*	17
				Jenkins, M.	12

<p>Jia, J.* 69</p> <p>Jian, J. 18, 19</p> <p>Jiang, S. 10</p> <p>Jin, K. 71</p> <p>Jin, N. 8</p> <p>Jin, W. 48</p> <p>Jin, W.* 35</p> <p>Johnson, A. N. 37</p> <p>Johnson, J. 25</p> <p>Johnson, J.* 33</p> <p>Johnson, S. D. 66</p> <p>Joly, Y. 15</p> <p>Jones, J. L. 12, 41, 53</p> <p>Jones, J. L.* 77</p> <p>Jørgensen, M. 37</p> <p>Jovanovic, Z. 66</p> <p>Jungwirth, N. 28</p> <p style="text-align: center;">K</p> <p>Kabir, A.* 43</p> <p>Kabos, P. 58</p> <p>Kakekhani, A. 62</p> <p>Kalasad, M. 19</p> <p>Kalasad, M.* 18</p> <p>Kalinin, S. 13</p> <p>Kaliyaperumal Veerapandiyam, V.* 21</p> <p>Kamiya, y. 50</p> <p>Kang, K.* 36</p> <p>Kaplan, W. D.* 7, 74</p> <p>Karateev, I. 66</p> <p>Karkare, S. 61</p> <p>Karpavicius, A. 35</p> <p>Karpisz, T. 56</p> <p>Karpov, D. 45</p> <p>Kaspar, T. 48, 72</p> <p>Kaspar, T.* 46</p> <p>Kato, K. 42</p> <p>Kaur Chhina, M.* 34</p> <p>Kawakami, R. K. 9</p> <p>Keavney, D. 46</p> <p>Kelley, K.* 13</p> <p>Khalsa, G.* 28</p> <p>Khan, A.* 44</p> <p>Khanbareh, H.* 76</p> <p>Khansur, N. 52</p> <p>Khatua, D. K. 40</p> <p>Kim, C. 27, 43</p> <p>Kim, C.* 33</p> <p>Kim, H. 17, 27</p> <p>Kim, J. 35</p> <p>Kim, N. 25</p> <p>Kim, Y. 36, 47</p> <p>Kim, Y.* 34</p> <p>Kintner, C. 57</p> <p>Kioupakis, E. 15, 64</p> <p>Kioupakis, E.* 49</p> <p>Kirby, B. 47</p> <p>Kitanovski, A. 10</p> <p>Klemm, R.* 69</p> <p>Kler, J.* 26</p> <p>Knappe, D. 77</p> <p>Koch, L. 55</p> <p>Kodumudi Venkatamaran, L. 43</p> <p>Koh, Y. R. 38</p> <p>Kolluru, V.* 31</p> <p>Komissinskiy, P. 27</p> <p>Kong, J. 40</p> <p>Koohfar, S. 46</p> <p>Kopyt, P. 56</p> <p>Kopyt, P.* 56</p> <p>Koshy, P.* 76</p> <p>Kotlarz, P. L. 61</p>	<p>Kotomin, E. A.* 61</p> <p>Kotsonis, G. N.* 64</p> <p>Kourkoutis, L. 9</p> <p>Kovacs, C. J.* 72</p> <p>Kowalski, B. 35</p> <p>Kozhakhmetov, A. 32</p> <p>Kozlowski, G. 71</p> <p>Kozlowski, G.* 72</p> <p>Kreisel, J. 21</p> <p>Krupka, J. 56</p> <p>Kulik, P.* 56</p> <p>Kumah, D. P. 9, 46</p> <p>Kumar, A. 9, 20</p> <p>Kuna, L. 36, 65</p> <p>Kuna, L.* 65</p> <p>Kutnjak, Z. 10</p> <p>Kutnjak, Z.* 21</p> <p>Kwon, O. 36</p> <p style="text-align: center;">L</p> <p>Ladonis, A. 73</p> <p>Lanagan, M. 17</p> <p>Lanagan, M.* 56</p> <p>Lany, S. 32</p> <p>Lapano, J. 66</p> <p>Lau, C. 11, 12, 71</p> <p>Lau, C.* 70</p> <p>Lau, D.* 55</p> <p>Lauter, V. 45</p> <p>Lazovic, G. 34, 41</p> <p>LeBeau, J. M. 9, 46</p> <p>LeBeau, J. M.* 20</p> <p>Lee, D. 58</p> <p>Lee, G.* 39</p> <p>Lee, H. 33, 45, 46</p> <p>Lee, H.* 45</p> <p>Lee, J.* 31, 32</p> <p>Lee, K. 36</p> <p>Lee, T. 39</p> <p>Lenz, E. 59</p> <p>Leonhard, T. 62</p> <p>Levchenko, S.* 60</p> <p>Levin, I.* 20</p> <p>Li, D. 71</p> <p>Li, F.* 41</p> <p>Li, J. 42</p> <p>Li, L. 18, 19</p> <p>Li, P. 62, 70</p> <p>Li, S. 12</p> <p>Li, S.* 70</p> <p>Li, Y.* 15</p> <p>Li, Z. 56</p> <p>Liao, Z. 46</p> <p>Liepe, M. 51</p> <p>Linthicum, W. 16, 62</p> <p>Lisenkov, S. 22</p> <p>Liu, X. 12</p> <p>Liu, Y. 43</p> <p>Liu, Y.* 12</p> <p>Liu, Z. 42</p> <p>Lofland, S. 22</p> <p>Lomeli, E. 8</p> <p>Long, C. 28</p> <p>Louis, L. 39</p> <p>Lowum, S. 18</p> <p>Lu, C. 41</p> <p>Lu, P. 19</p> <p>Lubbers, N. 39</p> <p>Lucero, M. 33</p> <p>Lucero, M.* 41, 54</p> <p>Luk, T. S. 16</p> <p>Luo, J. 38</p>	<p>Luo, J.* 74</p> <p>Lupascu, D. C. 14, 33</p> <p>Lupi, E. 11</p> <p>Lv, B. 12, 70</p> <p style="text-align: center;">M</p> <p>Ma, J. 51</p> <p>Ma, J.* 50</p> <p>Ma, Q. 40</p> <p>Maartense, I. 71</p> <p>Machado, P. 63</p> <p>Macutkevicius, J. 22</p> <p>Maglione, M. 21</p> <p>Mahato, D. K.* 10</p> <p>Maier, J. 61</p> <p>Majoros, M. 72</p> <p>Maksymovych, P. 63</p> <p>Maksymovych, P.* 50</p> <p>Malic, B. 10, 12, 53</p> <p>Maloney, J. G. 57</p> <p>Mangeri, J. 29, 65</p> <p>Mangum, J. 13, 27</p> <p>Manjon-Sanz, A. 12</p> <p>Mann, A. 33</p> <p>Mannix, D. 15</p> <p>Mantri, S.* 36, 44</p> <p>Manuel, M. 51</p> <p>Mao, T. 7</p> <p>Mao, Z. 71</p> <p>Marder, R. 74</p> <p>Mardilovich, P. 11, 52</p> <p>Maria, J. 16, 18, 20, 64, 65</p> <p>Marks, S. 15</p> <p>Markurt, T. 47</p> <p>Marlton, F. 37</p> <p>Marshall, P. 47</p> <p>Martin, L. W. 11</p> <p>Martin, M. 39</p> <p>Mastrikov, Y. 61</p> <p>Matavz, A. 23</p> <p>Mathur, S. 64</p> <p>Matson, J. 19</p> <p>Maune, H.* 27</p> <p>Maurya, D. 37</p> <p>May, S.* 49</p> <p>Mazza, A. 14</p> <p>McComb, D. W. 7, 18</p> <p>McComb, D. W.* 9</p> <p>McGarrahan, J.* 26</p> <p>McGuire, M. 63</p> <p>McQuade, R. 33, 41, 42, 52</p> <p>Mebane, D. S.* 23</p> <p>Mehmood, R. 76</p> <p>Mehta, A. 51</p> <p>Meisenheimer, P. B. 64</p> <p>Meisenheimer, P. B.* 15</p> <p>Mentzer, C. 22</p> <p>Menzler, N. H. 31</p> <p>Merkle, R. 61</p> <p>Mete, S. 7</p> <p>Metz, P. C. 73</p> <p>Michael, S. 70</p> <p>Mimura, K.* 42</p> <p>Minor, A. 8</p> <p>Mishra, A. 40</p> <p>Misra, S. 18, 19</p> <p>Misra, S.* 19</p> <p>Misture, S. T. 75</p> <p>Misture, S. T.* 73</p> <p>Mitic, V.* 34, 41</p> <p>Mofarah, S. 76</p> <p>Mohanty, B. C. 12</p>
--	--	---

Simchi, A.	43	Thompson, P.	15	Williams, R. E.	9, 18
Singamaneni, S.*	47	Thong, H.	42	Wilson, S. D.	47
Singh, D.	10	Tidrow, S.	43	Windl, W.	71
Singh, K.	34	Toledo, R. P.*	39	Winter, G.	56
Sitar, Z.	65	Tomko, J.	20, 38	Wolfley, S.	16
Skiba, E.	25	Toney, M. F.	13	Wollmershauser, J.	65
Skoropata, E.*	45	Toulouse, C.	21	Wood, V.*	67
Small, L.	53	Trassin, M.	13, 15	Woods-Robinson, R.	27
Smirnov, D.	11	Trassin, M.*	14	Woodward, P.*	69
Smith, K.*	28	Tretiak, S.*	60	Wu, H.	70
Smith, S.	12, 16, 19	Trickey, S.	51	Wu, J.	51
Sohn, C.	45	Trolier-McKinstry, S.	13	Wu, J.*	70
Sokolov, A.	56	Trolier-McKinstry, S.*	17	Wu, Y.	23, 24, 75
Son, Y.	33	Trout, A.	9	Wu, Y.*	24
Song, J.	16, 39	Truttmann, T.	61	Wuenschell, J.	55
Song, J.*	62	Tsuji, K.	75		
Soon, A.	32, 39	Turgut, Z.	72		
Sorenson, J.	35	Turriani, D.	72		
Sorenson, J.*	35			X	
Sorrell, C. C.	76			Xie, S. R.	50, 62
Spanier, J. E.	66	U		Xie, S. R.*	61
Spanier, J. E.*	65	Uberuaga, B. P.	60	Xin, C.	21
Spencer, M.	57	Uchida, H.	44	Xiong, H.	38
Spitaler, J.	21	Updegrave, A.*	57	Xiong, H.*	73
Spoerke, E.	53	Uršič, H.	52, 53	Xu, B.	43
Spoerke, E.*	53	Uršič, H.*	12	Xu, P.	74
Spreitzer, M.	23			Xu, Z.	37
Spreitzer, M.*	66	V			
Spurgeon, S. R.	46	Vasiliev, A.	66	Y	
Stanciu, L.	74	Vasiliev, I.	45	Yamaura, K.*	49
Stanek, C.	60	Vasudevan, R.	13	Yang, B.	51
Staruch, M. L.	22	Veber, P.	21	Yang, J. L.	76
Staruch, M. L.*	42	Veerabhadraiah, Y.	37	Yang, J.*	11
Steffes, J.	66	Velarde, G.*	11	Yang, O.	33
Steiner, S.	43, 55	Veljkovic, S.	34, 41	Yang, P.	35
Stemmer, S.	47	Venkatesh, R.	58	Yang, P.*	35
Stepanov, P.	71	Venkateshwarlu, S.	37	Yang, Y.	32
Sternlicht, H.*	7	Veras, S. E.	66	Yang, Z.	18, 20, 72
Stewart, G. R.	50	Vladimir, S. V.	14, 33	Yao, K.	36
Sumption, M. D.	72	Vlahovic, B.	41	Yazawa, K.*	44
Sun, W.	32			Ye, Z.*	22
Sun, X.	18, 19	W		Yildiz, B.*	24, 53
Sun, Y.	51, 68	Wada, S.	35	Yilmaz, D.	13
Sun, Z.	51	Walk, D.	27	Yoon, M.	30, 32
Sun, Z.*	11	Walker, J.	13	Yoon, S.	32
Sung, S.	15, 64	Wallis, T. M.*	58	Yoon, S.*	46
Sushko, P.	46	Wang, C.*	53	Yoshimura, M.*	30
Susner, M.	63, 72	Wang, G.*	51	Young, S.	22
Suter, A.	47	Wang, H.	18, 19	Yousfi, S.	14
Suvorov, D.	23, 66	Wang, J.	36	Yu, C.	56
Suzuki, Y.	70	Wang, J.*	76	Yu, H.*	47
Svirskas, S.	22	Wang, K.*	42	Yu, J.	56
		Wang, L.	72	Yu, L.	71
T		Wang, L.*	18	Yu, P.	64
Taddei, K.	70	Wang, Q.	10	Yuan, J.	71
Takamura, H.*	26	Wang, X.	8, 18, 19	Yuan, W.	40
Takamura, Y.	16	Wang, X.*	68		
Takeuchi, I.	40, 47	Wang, Y.	71	Z	
Takeuchi, I.*	47, 48	Wang, Z.	44, 64	Zachman, M.	9
Talapatra, A.	60	Wangoh, L.*	72	Zaengle, T.*	75
Talley, K.	27	Waqar, M.*	36	Zakutayev, A.	27, 67
Tan, A. Z.	24	Ward, T. Z.	14	Zakutayev, A.*	32
Tan, A. Z.*	32	Ward, T. Z.*	14	Zhang, B.	18
Tan, S.	32	Warzoha, R.	58	Zhang, B.*	18
Tan, X.	10	Watanabe, K.	11, 12, 71	Zhang, D.	18, 19
Taniguchi, T.	11, 12, 71	Webb, R. P.	37	Zhang, D.*	19
Tao, L.	63	Webber, K. G.*	52	Zhang, F.	12
Tavakoli Taba, M.	28	Weber, D.	71	Zhang, G.*	10
Telmer, M.	29	Wen, H.*	44	Zhang, L.	11, 32
Tempke, R.	57	Wexler, R.	59	Zhang, L.*	30
Thapa, S.	61	Weyland, F.	37	Zhang, M.	42
Thapa, S.*	48	Wilbur, J.	11	Zhang, Q.	10
Thiruvengadam, R.	69	Wildfire, C.	57	Zhang, S.	8, 20, 51
		Williams, L.	15, 64	Zhang, X.	19, 69
				Zhang, X.*	70

Author Index

Zhang, Z.	72	Zhou, H.	50, 72	Zhu, X.	20
Zhao, A.	69	Zhou, X.*	50	Zhu, Y.	71
Zhao, J.	41	Zhou, Y.	62	Zhuang, C.*	27
Zhao, Z.	71	Zhou, Y.*	73	Zhuang, J.	22
Zhelev, N. Z.	27	Zhu, D.	29	Zhuk, M.	76
Zheng, D.*	37	Zhu, J.	60	Zlobin, A.	72
Zhi, Y.	77	Zhu, L.	51	Zou, K.*	68
Zhou, F.	71	Zhu, W.	17	Zupancic, M.*	47