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2022 Conference on Electronic Materials and Applications (EMA 2022)

ABSTRACT BOOK

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Introduction

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How to Use the Abstract Book

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

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Wednesday, January 19, 2022

Plenary Sessions

Plenary Session I

Room: Orange A
Session Chair: Jennifer Andrew, University of Florida

8:40 AM

(EMA-PLEN- 001-2022) Solution Processed Nanoporous and Nanocrystal Based Magnetoelectric Materials

S. Tolbert*[1]

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Here, we examine multiple ways to control magnetism in solution processed nanostructured materials using an applied bias. We begin with traditional strain coupled multiferroics, and consider two systems. The first is a nanoporous magnetic network produced using polymer templating of sol-gel oxides. The pores are then conformally filled with the a ferroelectric using atomic layer deposition to produce a three-dimensional composite. We find the largest multiferroic response in materials with partly filled pores, emphasizing the role of residual porosity in controlling the elastic behavior and the multiferroic coupling. We next consider switching in monolayer nanocrystal arrays, showing that nanocrystals can be reversibly switched from a superparamagnetic state, which has no time-averaged magnetic moment, to a ferromagnetic state using an applied bias. Finally, we explore a new type of material, termed granular multiferroics, where exchange coupling between closely spaced magnetic nanocrystals can be modified by tuning the dielectric environment around the nanocrystals using either temperature or an applied electric field. In this work on nickel nanocrystals coupled to a soft ferroelectric, field dependent changes in magnetism are observed in the vicinity of the ferroelectric Currie temperature, indicating that magnetism in nanocrystal arrays can indeed be tuned using dielectric changes.

S1: Characterization of Structure–Property Relationships in Functional Ceramics

Advances in Scattering, Imaging, and Analytical Techniques

Room: Magnolia A
Session Chairs: James LeBeau, Massachusetts Institute of Technology; David McComb, The Ohio State University

10:00 AM

(EMA-001-2022) Towards characterization of the evolution of an electroceramic grain boundary network during thermal processing by in situ scanning transmission electron microscopy (Invited)

W. Bowman*[1]; J. L. Wardini[1]

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

Advanced electron microscopy characterization has enabled many studies on grain boundary (GB) structure-chemistry-property relationships in ceramics. However, establishing such relationships under dynamic and/or operating conditions remains limited due to the challenges of simultaneously characterizing ceramic GBs and functional properties, particularly if the system is evolving with time. This talk focuses on our recent work on determining a relationship between GB network characteristics (grain size, GB atomic structure, and local defect chemistry) and electrical resistance in a mixed ionic-electronic conducting (MIEC) oxide during the formation and evolution of GB networks. We have monitored structural (grain size, crystal structure) and chemical information (elemental distribution, and bonding environment) by in situ scanning and transmission electron microscopy (S/TEM) imaging and spectroscopy during thermal processing and have attempted to correlate this with temperature dependent electrical measurements. Looking forward, we are also developing an automated workflow capable of detecting the loci of GBs in a polycrystalline TEM specimen and applying localized STEM characterization.

10:30 AM

(EMA-002-2022) Evolution of polar domains with epitaxial strain in relaxor-ferroelectric PMN-PT thin films

A. Kumar*[1]; J. Kim[2]; L. W. Martin[2]; J. LeBeau[1]

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. University of California, Berkeley, Materials Science and Engineering, USA

Relaxor ferroelectrics, such as $PbMg_{1/3}Nb_{2/3}O_3$-$PbTiO_3$ (PMN-PT), exhibit nanoscale polar domain structures, which are challenging to control through composition and/or heat treatments alone. Recently, strain tuning of the polar structure and relaxor behavior of PMN-PT thin films has been demonstrated. The precise structural origins of the modified behavior, however, remain elusive. Here, we use scanning transmission electron microscopy (STEM) to probe the atomic structure of PMN-PT thin films with varying magnitudes of epitaxial compressive strain provided by the substrates during pulsed laser deposition (PLD). We use simultaneous annular dark field (ADF) and integrated differential phase contrast (iDPC) imaging to capture the cation and anion sublattices that are then used to reveal the correlation between the polar structure and local chemistry across epitaxially strained samples. Further, inhomogeneities such as chemical order, octahedral distortion order, and octahedral tilt order are quantified for the epitaxially strained samples, which reveals a complex relationship between these inhomogeneities, strain, and thin film thickness.

10:45 AM

(EMA-003-2022) Atomically resolved intermediate phase in sodium niobate

H. Ding*[1]; N. Hadaeghi[1]; E. Adabifiroozjaei[1]; L. Carstensen[1]; T. Jiang[1]; W. Donner[1]; H. Zhang[1]; H. Kleebe[1]; L. Molina-Luna[1]

1. Technical University Darmstadt, Materials Science, Germany

Antiferroelectrics have attracted worldwide attention for its great potential in energy storage devices due to its superior phase transition behavior i.e., that the antiferroelectric (AFE) and ferroelectric (FE) states can be mutually switched manipulated by an electric field. However, the reversible phase transition is rarely observed in the prototype AFE sodium niobate ceramics and the structural transformation involved during the transition is insufficiently investigated until now. Here, atomic resolved structures of AFE and FE phases in sodium niobate ceramics are explored by (scanning) transmission electron microscopy techniques. The straight-line features in the domain morphology known as antiphase boundaries can be observed in both states and may function as intermediate phase during the AFE-FE transition. This phase is found to have a 2-fold structure with non-polarity. DFT calculations further validates that the 2-fold intermediate phase has a very close but slightly higher free-energy than P and Q phases with a difference by 29 and 33 meV/f.u., respectively.

11:00 AM

(EMA-004-2022) Spatially Mapping Mechanical & Thermal Properties of Epitaxially-Grown Graphene with Sub-Micron Lateral Resolution

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We present measurements of the topographical, mechanical and thermal properties of 2D materials, acquired simultaneously pixel-by-pixel at the nanoscale through an innovative, laser-based scanning probe microscopy (SPM) platform. This platform leverages the operating principles of atomic force microscopy (AFM) and frequency-domain thermoreflectance (FDTR), where through active, laser-based heating of an AFM probe, unique maps of thermoreflectance data down to 10s of nanometers are generated that enable the local assessment of property variation and/or correlation with the defect structure of the material. Mechanical and thermal properties are acquired via either on or off-resonance operation in contact-mode, respectively; the former acquired via an approach similar to contact resonance microscopy, though using tip temperature (via thermoreflectance) as the measurable quantity instead of cantilever oscillation amplitude. Measurements conducted on epitaxially-grown graphene, as well as graphene-encapsulated, 2D layers of silver grown via Confinement Heteroepitaxy (CHet) are presented and discussed to highlight current capabilities, as well as plans for further development. This capability represents an important advancement in thermal metrology, enabling sub-micron lateral resolution not possible with diffraction-limited optical approaches.

11:15 AM

(EMA-005-2022) Measuring Atomic Scale Magnetization in a Metallic Antiferromagnet via 4D-STEM (Invited)

K. Nguyen[1]; J. Huang[1]; M. Karigerasi[1]; K. Kang[1]; A. Schleife[1]; D. Cahill[1]; D. Shoemaker[1]; J. Zuo[1]; P. Huang*[1]

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

The development of fast direct electron detectors for scanning transmission electron microscopy (STEM) is enabling new, atomic scale measurements of the functional properties of materials. In our work, we demonstrate a combination of experimental and computational four-dimensional (4D)-STEM to image the local magnetization in Fe_2As, a metallic antiferromagnet. Using a combination of quantum mechanical electron scattering simulations and experimental data gathered using the latest generation of electron detectors, we show how the weak scattering signals from magnetism can be isolated from convergent beam diffraction patterns and used to measure the direction and magnitude of the local magnetization. We obtain 6 Å resolution in Fe_2As, indicating new applications for 4D-STEM to probe the magnetic structure of antiferromagnets, promising systems for fast, dense computer memories because of their low magnetic susceptibilities and terahertz switching frequencies.

11:45 AM

(EMA-006-2022) Autonomous experiment in the electron microscope guided by actively learning structure-property relationships in STEM-EELS

K. M. Roccapriore*[1]; S. Kalinin[1]; M. Ziatdinov[1]

1. Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, USA

Local electronic properties of materials are observable in the scanning transmission electron microscope (STEM) by electron energy loss spectroscopy (EELS). If the electron source is sufficiently monochromated, this further allows to map optical and even vibrational modes at the nanoscale, making STEM-EELS an excellent tool for exploring emergent quantum materials, probing plasmonic and phononic properties, and mapping ferroic and charge density wave systems, among many other nanoscale systems. Largely overlooked but buried within operator experience is the relationship of the structural information, e.g., annular dark field (ADF) images, to the EEL spectra. The enormous parameter space available in the STEM is only partially sampled where specific regions in space are chosen based on operator knowledge. Recent machine learning methods such as Gaussian Processes (GP) and Bayesian Optimization (BO) have begun to enter the microscopy scene as tools for automating experiments to select new locations for exploration but offer limited flexibility. We demonstrate a solution by combining the power of BO with neural networks in the form of deep kernel learning that transforms the microscope into a platform for autonomous microscopy and even physical discovery. Using this approach, we discover edge plasmon functionality in a relatively unexplored 2D material, $MnPS_3$.

12:00 PM

(EMA-007-2022) Quantifying Temperature Susceptivity of Electron Scattering in Scanning Transmission Electron Microscopy

M. Zhu*[1]; J. Hwang[1]

1. Ohio State University, Material Science and Engineering, USA

Phonons can greatly influence the trajectory of radiations and in turn, affect the outcome of any scattering experiment. This means a proper quantification may provide important guidance to measuring the temperature (T) of the material at the length scale equivalent to the size of the probe used in the scattering experiment. In this work, we report the sensitivity of electron scattering to sample T as a function of the scattering angle in scanning transmission electron microscopy (STEM). Unlike the scattering intensities at higher angle ranges that are known to be dominated by thermal diffuse scattering and expected to decrease with increasing T, the T sensitivity of the intensities at lower scattering angles has been less understood. In fact, our data reveal that the scattering intensities at low-to-intermediate angles show the opposite behavior, with the intensity increasing as the T increases, and the amplitude of the change is higher than that in high angle scattering. This trend was observed in position averaged convergent beam electron diffraction as well as the atomic-scale images reconstructed from 4-dimensional STEM. Based on the finding, we quantified the trend as a function of both T and the scattering vector, which provides important guidance toward realizing the T measurement of materials with high T precision and spatial resolution close to the atomic scale.

12:15 PM

(EMA-008-2022) In-Situ and In-Operando Study of Electrochemical Strain in MnO_2 nanosheet electrodes

M. N. Flint*[1]; P. Metz[1]; P. Gao[1]; R. Koch[1]; S. T. Misture[2]

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2. Alfred University, MSE, USA

The paper discusses the use of multiple in-situ/operando characterization tools to understand the behavior of exfoliated and re-assembled nanosheet electrodes. The nanosheets form low-density floccules upon self-assembly, yielding crumpled and wavy nanosheets with some limited restacking. In-situ and in-operando methods were applied to understand the effects of Mn^{3+} defects on the electrochemical behavior and to track the chemomechanical responses and consequently the charge cycling stability. In-situ/operando methods included X-ray total scattering, X-ray absorption spectroscopy, Raman spectroscopy, and electrochemical kinetic studies. The result is a description of the charging mechanism in high surface area MnO_2 nanosheet electrodes and related nanosheet oxides: reversible in-plane strains of up to 0.7% occur during charging, accompanied by a Mn^{4+} to Mn^{3+} without any significant interlayer strain response. Raman spectra support the scattering data and demonstrate a reversible increase in the number of Jahn-Teller distorted trivalent MnO_6 octahedra in the charged state. The

excellent cycling stability of the nanosheet electrodes vs. bulk solids is attributed to the free space in the floccules and presence of interlayer water that allows electrochemically-driven expansion and contraction without degrading the charge transfer pathways and without microcracking the active electrode.

Addressing Open Questions in Functional Ceramics

Room: Magnolia A

Session Chairs: Hadas Sternlicht, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory; Abhijit Pramanick, City University of Hong Kong

2:00 PM

(EMA-042-2022) Probing the influence of defects and interfaces on the multiferroic behavior of layered Aurivillius phase thin films (Invited)

L. Colfer[2]; N. Bagués[3]; K. Moore[4]; E. O Connell[4]; S. Griffin[5]; M. Schmidt[2]; C. Downing[6]; V. Nicolosi[6]; U. Bangert[4]; M. Conroy[7]; D. W. McComb[8]; L. Keeney*[1]

1. Tyndall National Institute, University College Cork, Advanced Materials and Surfaces Group, Ireland
2. Tyndall National Institute, Ireland
3. The Ohio State University, Center for Electron Microscopy and Analysis, USA
4. Bernal Institute, University of Limerick, Department of Physics, Ireland
5. Molecular Foundry, Lawrence Berkeley National Laboratory, USA
6. Trinity College Dublin, Advanced Microscopy Laboratory & AMBER, Ireland
7. Imperial College London, Department of Materials, Royal School of Mines, United Kingdom
8. The Ohio State University, USA

Multiferroic materials intertwine ferroelectric and ferromagnetic properties, allowing for novel ways of manipulating data and storing information. The Aurivillius phase $Bi_6Ti_xFe_yMn_zO_{18}$ (B6TFMO) system is a rare example of a multiferroic displaying room-temperature behavior. To optimize properties and exploit B6TFMO for future memory storage applications, in this work, we use high resolution energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) in the aberration corrected STEM to understand the origin of these unique properties. We demonstrate how internal electrostatic strain and elastic energy differences within the layered Aurivillius structure effect alignment and partitioning of magnetic cations at bismuth oxide interfaces and defects. We reveal how electrostatic strain and elastic energy variations close to defect regions also influence the formation of exotic charged domain walls and polar vortices. Based on the results of these experiments, we will discuss the influence of sub-unit cell characteristics on the multiferroic properties of this intriguing system.

2:30 PM

(EMA-043-2022) Mechanical tailoring of dislocation density in $SrTiO_3$ at room temperature via cyclic loading

X. Fang*[1]; C. Okafor[1]; K. Ding[1]; X. Zhou[1]; K. Durst[1]; J. Rödel[1]

1. Technical University of Darmstadt, Germany

Dislocation-based functional properties such as electrical conductivity, thermal conductivity, and ferroelectric properties in oxides are attracting increasing research interest. A prerequisite for harvesting the dislocation-based functional properties in oxides requires successful introduction and control of dislocation density and arrangement without forming cracks, which is a great challenge due to the brittle nature of ceramics. Here, we report a simple method to mechanically tailor the dislocation density in single-crystal perovskite $SrTiO_3$. By using an indentation method with millimeter-sized Brinell (spherical) indenters, dislocation densities from 10^{10} m^{-2} to 10^{13} m^{-2} are achieved by increasing the number of indenting cycles. Depending on tip radius and indenting load, large plastic zones over hundreds of micrometers are created without forming cracks. The dislocation multiplication mechanisms are discussed, and the work hardening in the plastic zone is assessed by micro hardness measurement as a function of the dislocation density. This simple approach opens many new opportunities in the area of dislocation-based functional and mechanical studies.

2:45 PM

(EMA-044-2022) Small-scale mechanical characterization of $LiTaO_3$ and $LiNbO_3$ single crystals for SAW filters

M. Gruber*[1]; D. Kiener[2]; P. Supancic[1]; R. Bermejo[1]

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2. University of Leoben, Department of Materials Physics, Austria

The requirements on new materials used in mobile communications are driven by the demand for higher data transfer rates. Single crystalline piezoelectric materials such as $LiTaO_3$ and $LiNbO_3$ have thereby qualified as substrates for precise and efficient frequency filters and are consequently employed in the newest 5G mobile communication network standards. Crystal growth in specific orientations are usually pursued to ensure optimized functional properties. The question rises whether such orientations may withstand thermo-mechanical loading during qualification and/or service. In this work, biaxial strength measurements along with in-situ SEM fracture toughness experiments were performed on miniaturized specimens to investigate the mechanical performance of $LiTaO_3$ and $LiNbO_3$ materials. Atomistic modelling calculations supported the experimental results and provided recommendations for crystal orientations with enhanced mechanical properties. In addition, nanoindentation experiments and preliminary in-situ TEM tests showed onset of plastic deformation for specific loading scenarios. These findings at the micro-scale may be utilized in the fabrication of $LiTaO_3$ and $LiNbO_3$ materials of particular orientations with optimized structural and functional properties.

3:00 PM

(EMA-045-2022) Lightly Fe-doped Polycrystalline Strontium Titanate: Tracking Fe Valence Changes Upon Sintering

M. Knight*[1]; I. Reimanis[1]; A. Meyer[1]; J. Preusker[2]; W. Rheinheimer[3]

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2. Karlsruhe Institute of Technology, Germany
3. Forschungszentrum Juelich, Germany

Bulk polycrystalline strontium titanate with small amounts of Fe substituted for Ti is a model representative for acceptor-doped large bandgap electroceramics. This work investigates changes in Fe valence upon sintering for Fe doping concentrations of 0.2mol%, 0.5mol%, and 1.2mol%. X-ray diffraction and Raman spectroscopy confirm successful substitution; while DC magnetic susceptibility, electron paramagnetic resonance, and Mossbauer techniques are combined to identify paramagnetic Fe^{3+} and Fe^{4+} species. Negative exchange interactions suggest Fe acceptors segregate in the grain boundary regions.

3:15 PM

(EMA-046-2022) Point defect induced dipole moments in $KCa_2Nb_3O_{10}$ Dion-Jacobson layered perovskites

J. Kong*[1]; S. Nayak[3]; K. Co[3]; S. Nayak[4]; J. Wu[1]; A. Feteira[2]; B. Kevin A[5]; P. Alpay[3]; A. Pramanick[1]

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2. Sheffield Hallam University, United Kingdom
3. University of Connecticut, Department of Materials Science and Engineering, USA
4. Indian Institute of Technology Madras, Department of Physics, India
5. Advanced Photon Sourc, USA

Local structural distortions due to isolated atomic defects and defect complexes strongly affect the macroscopic properties of oxide ceramics. While characterization of local defect structures is more common in simple ABO_3 perovskites, unambiguous determination of the same in layered perovskites is more difficult due to their complex crystal structures. Here, we combined x-ray pair distribution function and density functional theory calculations to characterize the structure of cation-oxygen divacancy pairs in a $KCa_2Nb_3O_{10}$ Dion-Jacobson (D-J) layered perovskite. The current results imply that controlling the atomic defects can potentially lead to significant control of dielectric properties in D-J layered perovskites.

3:30 PM

(EMA-047-2022) Clarifying dislocation structures in strontium titanate using atomistic simulations

A. J. Klomp*[1]; L. Porz[1]; K. Albe[2]

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A couple of years ago, research into the deformation behavior of strontium titanate (ST) has sparked enthusiasm over the prospect of large plastic deformation in perovskite ceramics. In single crystals dislocation-based plasticity has unexpectedly enabled strains of almost 20%. Since then, a multitude of research efforts have deformed single-crystals and polycrystalline ST in order to understand the prerequisites for plasticity and the structural features of the relevant dislocations. Yet, the intensive debate has so far been limited by the narrow scope of processing conditions, dislocation types or boundary conditions employed. In a systematic overview, we have used atomistic simulations to model a variety of dislocation types that were claimed to be relevant to dislocation-based plasticity in ST. First, we confirm the importance of dislocation splitting for the mobility of dislocations. Second the influence of non-stoichiometry and associated charging of the dislocation core on its structure are revealed. Third, the relevance of the dislocation line direction and its character – edge, screw, or mixed – are discussed in detail. All these features should determine if a dislocation can contribute to macroscopic plasticity in ST. By the simulations of dislocation propagation under applied load, we show that the motion of dislocation is indeed a result of these factors.

Advances in Connecting Local and Global Structure to Properties

Room: Magnolia A

Session Chairs: Igor Levin, NIST; Chris Fancher, Oak Ridge National Lab

4:00 PM

(EMA-048-2022) Neutron diffraction studies of phase transitions in improper and incommensurate ferroelectrics (Invited)

F. D. Morrison*[1]

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Powder x-ray diffraction remains the primary technique for structural characterisation of ferroelectric oxides, however, its relative insensitivity to light oxide ions means that it often does not reveal many subtle structural changes which are manifested in the electrical response. In this regard, powder neutron diffraction (PND), is a powerful tool for understanding subtle structure-property relations. This will be demonstrated in the context of two recent studies: 1) The hexagonal tungsten bronze, $CsNbW_2O_9$, undergoes an improper ferroelectric cell tripling below $T_C \sim 1100$ K reminiscent of the hexagonal rare earth manganites and also exhibits the same meandering domain microstructure. However, PND explicitly shows that the symmetry breaking in $CsNbW_2O_9$ at T_C does not involve tilting and so the mechanism is electronically-driven, in contrast to the geometrically- (tilt-)driven mechanism of the manganites. 2) The geometric ferroelectric $LaTaO_4$ is a n = 2 member of the so-called $A_nB_nO_{3n+2}$ Carpy-Galy phases and is one of the simplest examples of a proper geometric ferroelectric. PND, complimented by electron microscopy, allowed identification of an intermediate incommensurately modulated phase. The appearance of this phase explains a previously unidentified dielectric anomaly and region of uniaxial negative thermal expansion.

4:30 PM

(EMA-049-2022) Integration of $BaZrO_3$-Co vertically aligned nanocomposite on mica substrates towards flexible spintronics

J. Liu*[1]; X. Wang[1]; X. Gao[1]; H. Wang[1]; B. Zhang[1]; D. Zhang[2]; M. Kalaswad[1]; J. Huang[1]; H. Wang[3]

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Integration of functional thin films with anisotropic physical properties onto flexible substrate is of great importance for future flexible electronics applications. In this work, $BaZrO_3$(BZO)-Co vertically aligned nanocomposite thin films have been integrated onto flexible mica substrate by using pulsed laser deposition. Microstructure characterization shows high quality growth of Co nanopillars in the BZO matrix. Tunable, anisotropic ferromagnetic properties of the films have been achieved by controlling the film thickness and the aspect ratio of Co nanopillars. The bending stability test was carried out under different bending conditions and cyclic bending to explore the physical properties of the films. The successful integration of BZO-Co on mica substrates opens a way for future flexible spintronics and device integration.

4:45 PM

(EMA-050-2022) Variations in the electronic structure and spin states in $La_{1-x}Sr_xCoO_3$

J. Shi*[1]; H. Zhang[2]

1. Xiamen University, Department of Chemistry, China
2. Xiamen University, College of Chemistry and Chemical Engineering, China

The $La_{1-x}Sr_xCoO_3$ (LSCO) have been attracting numerous attentions owing to their emergent characteristics with increase in hole doping, e.g., giant magnetoresistance (MR) effects, etc. However, the

electronic structure and spin states in $La_{1-x}Sr_xCoO_3$ remain debated, owing to the multiple interactive degrees of freedom including spin, orbital, lattice and defects. Here we present a investigation on the electronic structure and spin states across the hole-induced metal-insulator transition in $La_{1-x}Sr_xCoO_3$. High quality epitaxial films with Kiessig fringes were grown by PLD. In x= 0-0.5, the resistivity of $_xSr_xCoO_3$ experiences a gradual decrease from insulating to metallic with MIT point at x=0.2. However, an opposite trend is shown in x=0.5-1, raising questions among the Co valency and spin. Combing XPS, XAS and DFT calculations, we come to the following discoveries: The Co valency experiences a consistent increase from +3 to +4, with linear growth in x=0-0.5 and a gradually slowing growth in x=0.5-1. The slowing growth is attributed to the increase of O vacancies attributed to the thermodynamic instability of Co^{4+}. $LaCoO_3$ shows a combined spin state with low-spin Co^{3+} and high-spin Co^{3+}. With increased Sr^{2+} doping, a combination of high-spin Co^3 and high-spin Co^{4+} is becoming dominant. After x>0.5, the intermediate-spin Co^{4+} appears and finally become the main states with high-spin Co^{4+}.

5:00 PM

(EMA-051-2022) Atomic mechanisms for phase transitions in antiferroelectric $NaNbO_3$ studied by X-ray and neutron scattering

C. S. Htet*[6]; S. Nayak[2]; J. Kong[1]; L. Jue[3]; A. M. Manjon Sanz[3]; F. Marlton[4]; D. Sørensen[5]; M. Jørgensen[5]; A. Pramanick[1]

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Sodium niobate ($NaNbO_3$ or NN) exhibits transitions between several ferroelectrics (FE) and antiferroelectric (AFE) phases at different temperatures. Recently, solid-solutions of NN with stabilized AFE phases(s) have gained attention for energy-related applications. A better understanding of the atomic mechanisms responsible for AFE/FE phase transitions in $NaNbO_3$ can enable a more rational design of its solid-solution systems with tunable structural properties. Here, we have investigated atomic structural changes in NN using a combination of X-ray/neutron diffraction and neutron pair distribution function (PDF) analyses. Rietveld refinement of the X-ray/neutron diffraction patterns indicated a coexistence of the FE Q ($P2_1ma$) and AFE P (Pbcm) phases for temperatures 300-615 K, while PDF analysis indicated that the local structure (r < 8 Å) has a $P2_1ma$ symmetry. Moreover, we observed larger octahedral distortion for the local structure as compared to the average structure. Above 615 K, the average structure transitions to an AFE R phase (Pmmn), while PDF analysis indicates an increased disordering of local octahedral distortions and Na displacements. These results indicate that the average P/Q/R phase transitions in NN can be described as a result of complex ordering of octahedral tilts at the nanoscale, which are possibly coupled to the off-centered displacements of the Na atoms.

5:15 PM

(EMA-052-2022) Role of Cooperative Factors in the Photocatalytic Activity of Ba and Mn Doped $BiFeO_3$ Nanoparticles

A. Dubey*[1]; A. Schmitz[2]; S. V. Vladimir[1]; G. Bacher[2]; D. C. Lupascu[1]; M. E. Castillo[1]

1. University of Duisburg-Essen, Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), Germany
2. University of Duisburg Essen, Werkstoffe der Elektrotechnik and CENIDE, Germany

The escalated photocatalytic (PC) efficiency of the visible light absorber Ba doped $BiFe_{0.95}Mn_{0.05}O_3$ (BFM) nanoparticles (NPs) as compared to $BiFeO_3$ (BFO) NPs is reported for the degradation of the organic pollutants rhodamine B and methyl orange. 1 mol % Ba doped-BFM NPs degrade both dyes within 60 and 25 minutes under UV+visible illumination, respectively. The Ba and Mn co-doping up to 5 mol % in BFO NPs increases the specific surface area, energy of d-d transitions, and PC efficiency of the BFO NPs. The maximum PC efficiency found in 1 mol % Ba doped BFM NPs is attributed to a cooperative effect of factors like its increased light absorption ability, large surface area, active surface, reduced recombination of charge carriers, and spontaneous polarization to induce charge carrier separation. The 1 mol % Ba and 5 mol % Mn co-incorporation is found to be the optimum dopant concentration for photocatalytic applications. These properties of co-doped BFO NPs can, e.g., be exploited in the field of water splitting.

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

Advanced Electronic Materials, including Ferroelectric, Piezoelectric, Dielectric, Electrostrictive, and Pyroelectric Materials I

Room: Citrus A

10:00 AM

(EMA-009-2022) Design of Actuators Based on Relaxor-Ferroelectric Crossover (Invited)

D. Cann*[1]; S. Gupta[1]; B. Gibbons[1]; P. Mardilovich[2]

1. Oregon State University, USA
2. aixACCT Systems GmbH, Germany

Advancements in piezoMEMS technology requires new high-performance actuator materials that are designed to meet several challenging requirements. For example, actuator materials must exhibit large electromechanical strains over a wide temperature range at relatively low voltages, must maintain actuation performance over more than 10^{11} cycles, and the processing of these materials in thin film embodiments must be fully compatible with other components in the MEMS package. Ferroelectric piezoelectric materials such as PZT have been widely employed for these applications, however the present work explores a novel family of materials that utilizes a relaxor-ferroelectric crossover mechanism to generate large electric-field induced strains. With this approach, the ferroelectric state transitions into the relaxor state due to the disruption of long-range dipole order through chemical substitutions. Upon application of an external electric field, the ferroelectric state is regained resulting in large, fully reversible strain with effective normalized strain coefficients as high as 600 pm/V. This work will present data demonstrating the viability of the crossover mechanism as an actuator material, with an emphasis on the manipulating the relative stability of the ferroelectric and relaxor states.

10:30 AM

(EMA-010-2022) Critical processing parameters for sputtered ferroelectric AlBN thin films

J. Hayden*[1]; J. Maria[1]

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

Newly discovered wurtzite-structured ferroelectrics including $Al_{1-x}Sc_xN$, $Al_{1-x}B_xN$, and $Zn_{1-x}Mg_xO$ offer great potential as CMOS compatible ferroelectric materials for non-volatile memory applications. However, thin film growth challenges and degraded ferroelectric properties at small film thicknesses hinder integration of these materials into functional devices with low operating voltages and acceptable leakage currents. This work investigates thickness scaling of the ferroelectric properties of c-axis oriented $Al_{1-x}B_xN$ thin films prepared by reactive magnetron co-sputtering. Film structural properties, surface morphology, and ferroelectric properties are studied by x-ray diffraction, atomic force microscopy, and polarization hysteresis measurements, respectively, as a function of film thickness. Choice of bottom electrode material and its surface roughness, built-in stress, and degree of orientation are found to be influential in surpressing alternatively oriented grains (AOGs) and improving film texture at small thicknesses. For films grown on Si substrates a plasma cleaning proceedure followed by AlN seed layer was necessary to improve bottom electrode texture and eliminate AOGs.

10:45 AM

(EMA-011-2022) Full depth Crystallization of (Ba,Sr)TiO_3 thin films at 300°C with laser and their microwave range characteristics

K. J. Raju*[1]

1. University of Hyderabad, Physics, India

Only crystalline ferroelectrics give their special properties but most of the oxide ferroelectrics crystallize only at 700°C in thin film form which is not compatible with nanoelectrinics. In this process films are deposited at 300°C and then they were subjected to an expanded laser beam at the same temperature. It was found that the crystallization happens from the top and that too only for a depth of 120nm. Hence this process was repeated till a thickness of 600nm was reached which is good for applications involving tunable microwave devices. The microwave range characteristics of the films were studied using patterned test structures. It is found that the films gave signs of good crystallization with XRD and Laser Raman spectra with well defined peaks with a steady band edge narrowing leading finally to band gap value close to that of single crystal with increase in laser annealing duration till some optimum value. However their microwave range dielectric properties were quite different from that of the conventionally crystallized films, with tunability of 34% while the conventional films gave about 60% tunability at microwave frequencies. A TEM analysis showed that the annealed films consists of islands of crystallites surrounded by an amorphous matrix of the material which explains the observation and shows that full crystallization is the sulution.

11:00 AM

(EMA-012-2022) Effect of B-Site Cation Ratio on Properties of Sn-modified PZT 95/5

E. Neuman*[1]; N. Anselmo[1]; A. Meyer[1]; C. Diantonio[1]; M. Rodriguez[1]; R. Torres[1]; B. Brane[1]

1. Sandia National Laboratories, USA

The effect of varying B-site cation ratios on the microstructure and electrical properties of Sn-modified PZT 95/5 compositions was investigated. Dense material was prepared by the solid-state synthesis route using traditional ceramic processing methods. The Ti:Zr,Sn ratio was varied from 0.05 to 0.07 and Nb:Ti,Zr,Sn ratio was varied from 0.015 to 0.020 The sintered material was characterized using ICP-OES, XRD, and SEM/EDS, impedance spectroscopy, P-E-ε hysteresis looping, and pressure induced depolarization. The effect of composition on the processing, properties, and FE-AFE phase transition will be discussed. Sandia National Laboratories is a multimission 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-NA000352

11:15 AM

(EMA-013-2022) Understanding Thermal Transport between Amorphous GeTe and Crystalline GeTe (Invited)

B. F. Donovan*[1]; T. Gray[1]; R. J. Warzoha[1]; J. Champlain[2]; L. Ruppalt[2]; A. Giri[3]

1. United States Naval Academy, USA
2. Naval Research Labs, USA
3. University of Rhode Island, USA

Germanium Telluride (GeTe) is a phase change material that is of critical importance to a variety of fields including novel phase change-based memory in microelectronics. The phase change in this material is a thermally driven process and so understanding the heat flow dynamics, especially in small scale configurations, is of the utmost importance. In this study, we utilize Time Domain Thermoreflectance in order to measure the thermal properties of thin films of GeTe in crystalline and amorphous forms. With careful sample configuration, we aim to understand the physics behind thermal transport between amorphous and crystalline GeTe. Given our sample configuration and findings, these results help lend insight in general into the nature of amorphous thermal carriers.

11:45 AM

(EMA-014-2022) Acoustic Energy Harvesting of Piezoelectric 1-3 Composites

J. Figueroa[2]; M. Staruch*[1]

1. U.S. Naval Research Laboratory, USA
2. St. Mary's University, Physics, USA

Acoustic energy is an often overlooked but increasingly prevalent source of ambient energy that could be scavenged to power a wide range of devices. Piezoelectric materials are often used, but the tradeoff between acoustic impedance matching and amount of piezoelectric active material has not previously been investigated. In this work, commercially available 1-3 Dice and Fill composites with various fill factors (25%, 45%, and 65% of $Pb(Zr,Ti)O_3$) were tested using an impedance tube and then modeled using the KLM equivalent circuit model, and the results compared. As expected, the higher amount of ceramic material results in a higher absorption coefficient for the acoustic power. Experimentally, the higher fill factors also resulted in a higher peak output power at all dB levels, reaching a maximum of 115 nW (84 nW/cm^3) at 111 dB_{SPL} for the 65% fill sample. In the model, the 25% fill factor actually shows the highest expected output power, but this discrepancy is most likely due to a lowered piezoelectric coefficient during testing due to clamping conditions.

12:00 PM

(EMA-015-2022) Synthesis and Characterization of a Novel Ferroelectric Solid Solution

T. Rowe*[1]; M. Dolgos[1]

1. University of Calgary, 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), a region of phase instability determined by chemical composition, but the continued use and disposal of lead containing compounds has led to the desire for alternatives whether they have reduced lead content or are altogether lead-free compounds. Thus, the main goal for this project was to utilize lead titanate as an end member to discover a novel reduced lead solid solution displaying a similar MPB to PZT, meaning a

rhombohedral to tetragonal structural transition. This solid solution was therefore synthesized using traditional solid state synthesis techniques and multiple experiments were run to fully characterize the structure and property relationships. Thus far, results show a high Curie temperature ferroelectric material with similar structural changes to PZT leading to interesting electrical properties with potential for multiple applications through future research.

Advanced electronic materials, including ferroelectric, piezoelectric, dielectric, electrostrictive, and pyroelectric materials IIAdvanced Electronic Materials, including Ferroelectric, Piezoelectric, Dielectric, Electrostrictive, and Pyroelectric Materials II

Room: Citrus A

2:00 PM

(EMA-053-2022) Enhanced piezoelectric response and superior temperature stability of tetragonal (Ba, Ca)(Zr, Ti)O_3 textured ceramics (Invited)

Q. Kou[1]; B. Yang[1]; Y. Sun[1]; S. Yang[2]; L. Liu[1]; H. Xie[1]; S. Zhang[3]; F. Li[2]; Y. Chang*[1]

1. Harbin Institute of Technology, China
2. Xi'an Jiaotong University, China
3. Nanjing University, China

Lead-free ceramics with both high piezoelectric response and good temperature stability are demanded for electromechanical conversion devices. Unfortunately, owing to coexistence of polymorphic phases near room temperature, enhanced piezoelectric properties were usually achieved with occurrence of strong temperature dependence in modified $BaTiO_3$ ceramics. In this work, both $<001>_c$- and $<111>_c$-oriented tetragonal (Ba, Ca)(Zr, Ti)O_3 ceramics with texture degrees F>90% were synthesized via templated grain growth. Interestingly, the ceramics textured along the $<001>_c$ polar axis show much higher microscopic and macroscopic piezoelectric properties than those with nonpolar $<111>_c$ texture, indicating an "extender" ferroelectricity nature. Compared with non-textured samples, the $<001>_c$-oriented ceramics exhibit ~1.6 times higher piezoelectric strain, 4.4 times higher piezoelectric figure of merit, and better temperature stability (strain variation ≤ 5% between RT and 110°C). Such thermally stabilized strain response can be mainly attributed to wide temperature range of tetragonal phase and stable domain structure. This work provides a promising route for further developing lead-free piezoceramics with high and temperature-insensitive performance, which can broaden their application areas.

2:30 PM

(EMA-054-2022) Role of A-site cation off-centering in perovskite pseudo-cubic structure of Bi-based piezoelectrics. (Invited)

S. Kim*[1]; H. Nam[2]; I. Fujii[2]; S. Ueno[2]; c. moriyoshi[1]; Y. Kuroiwa[1]; S. Wada[2]

1. Hiroshima University, Japan
2. University of Yamanashi, Japan

Bi-based lead-free system is one of replacement for lead-based material. An interesting property of the Bi-based lead-free ceramics is that maximum piezoelectric response is exhibited meanwhile the ferroelectric property decreasing and dielectric constant increasing trend. This phenomenon is related to material softening. Although the material softening can be easily seen in the Bi-based lead-free piezoelectric materials, and the origin of the material softening in the $BiFeO_3$-$BaTiO_3$ (BF-BT) is unclear. In this study, the origin of the material softening in BF-BT was investigated. The material softening was exhibited in the wide composition range, and the maximum material softening was exhibited at the composition of 0.7BF-0.3BT. The synchrotron radiation X-ray diffraction patterns of the 0.7BF-0.3BT ceramics showed single, undivided diffraction peaks, which suggested the material had cubic-like symmetry. Rietveld refinements indicated that the crystal structure was indeed rhombohedral structure at 300K with Bi ion off-centering. Structural parameters such as lattice constant, bond-length, and Bi off-center displacement were calculated from the final structure refinement results. The maximum Bi off-center displacement and minimum Bi-O bond-length were observed in the 0.7BF-0.3BT ceramics. More detail of the results will be discussed in the presentation.

3:00 PM

(EMA-055-2022) Novel family of n-type oxide thermoelectric materials based on $La_{1.5-x}Eu_xSr_{0.775}TiO_{3-\delta}$ made using an ionic liquid synthesis

S. Mudd*[1]; R. Boston[2]; E. A. Casanas[1]

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

Thermoelectric materials convert waste heat energy into electricity. A high power factor and low thermal conductivity are required to enhance the thermoelectric figure of merit, ZT, which are often mutually exclusive characteristics in intrinsic materials. Oxides are a much cheaper alternative to current materials used in commercial thermoelectric devices but often suffer from high thermal conductivity due to strong covalent bonds. $Sr_{0.775}La_{0.15}TiO_3$ has an impressive power factor but its high thermal conductivity makes the ZT too low for commercial interest. Here we present a novel family of n-type oxide thermoelectric materials based on $La_{1.5-x}Eu_xSr_{0.775}TiO_{3-\delta}$ made using an ionic liquid synthesis. The ionic liquid synthesis used here enables full cation mixing during synthesis, resulting in a fully homogeneous product (even with very low dopant levels) and as such requires lower calcination temperatures than conventional solid state methods (800 °C VS 1200 °C). We observed that small amounts of europium cause a contraction in the lattice parameter and reduce the thermal conductivity.

3:15 PM

(EMA-056-2022) Reactive cold sintering of (Na,Ba)(Nb,Ti)O_3

J. Andrews*[1]; R. Boston[1]

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

As the world becomes more automated and connected there has been rapid growth in the number of electronic devices and ~3 trillion ceramic capacitors are manufactured every year. Conventional sintering methods at high temperatures account for up to 35% of the thermal energy requirements in the production of ceramic components. Reducing sintering temperatures could have a number of benefits in capacitor manufacture, including enabling the use of a wider range electrode materials and new, previously incompatible material combinations. Whilst barium titanate is still the material of choice for multilayer capacitor manufacture, in order to optimise properties to fit X7R standards a variety of dopants (often expensive or rare earth elements) are often required. Combining materials with contrasting dielectric properties has been demonstrated as a method to improve the temperature sensitivity of the permittivity and potential avoid the issue of dopants. This work demonstrates the use of a reactive cold sintering method to densify a number of compositions in the (Na,Ba)(Nb,Ti)O 3 system and aims to tailor the temperatures stability of dielectric properties through the creation of mixed/layered components.

4:00 PM

(EMA-057-2022) Electrical Property Modification and Physical Mechanism Investigation of KNN-based Lead-free Piezoceramics (Invited)

T. Zheng*[1]

1. Sichuan University, China

Piezoelectric ceramics are widely used in electronic devices due to their excellent electromechanical conversion. Although lead-based piezoelectric ceramics have excellent electrical properties, the large amount of toxic lead element cause damage to human health and serious environment pollution. Therefore, the development of lead-free piezoceramics has become the focus of current research. Among all kinds of lead-free systems, potassium sodium niobate [$(K_{0.5}Na_{0.5})NbO_3$, (KNN)] ceramics are considered to be the most likely candidates to replace lead-based materials due to their superior electrical properties and high Curie temperature. However, the properties of KNN-based ceramics still have problems such as weak piezoelectricity, poor temperature stability, sensitive sintering process, and lack of understanding of high performance structural origin. In view of the above problems, this paper takes the phase boundary construction as the starting point, systematically studies the KNN-based ceramics from piezoelectricity, physical mechanism, and temperature stability, including the relationship among composition modification, phase boundary types, and electrical properties; the structural origin of high performance of KNN-based lead-free ceramics; and the relationship between structure and temperature stability of KNN-based lead-free ceramics.

4:30 PM

(EMA-058-2022) Phase-field modeling of domain structure and piezoresponse in ferroelectric nanotubes (Invited)

S. Zhuang[1]; M. Li[1]; M. Zhang[1]; A. Ross[1]; J. Hu*[1]

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

Ferroelectric nanotubes represent an exciting material platform for exploring new topological polar states, physics and functionalities, due to its large vertical-to-lateral aspect ratio, curvature, and surface-to-volume ratio that are not simultaneously available in planar thin film and nanodots. In long nanotubes, polarization configuration may extend not only in the plane but also into the vertical dimension, thus may allow accommodating a broader spectrum of possible polar states (analogous to the case in the emergent field of three-dimensional nanomagnetism). In this talk, the speaker will present a phase-field model that can accurately and efficiently simulate the influence of dimension, orientation, composition, surface tension, substrate, surround media, and electrodes on the polarization domain structure and the associated piezoresponse in perovskite oxide ferroelectric tubes. The simulation results on (001) $Pb(Zr_{1-x}Ti_x)O_3$ (x=0.48, 0.8) nanotubes predict the presence of unique topological domain states such as periodic patterns of flux-closure and anti-flux-closure along the vertical dimension as well as large surface piezoresponse with d_{33}>1000 pm/V. The phase-field model can also be extended to simulate composite ferroic nanotubes comprising dissimilar ferroic materials.

5:00 PM

(EMA-059-2022) Dielectric properties of hybrid perovskites

D. C. Lupascu*[2]; A. Karabanov[1]; Y. Jin[1]; A. Farooq[1]; K. Winkler[3]; N. Benson[3]

1. University of Duisburg-Essen, Institute for Materials Science, Germany
2. University of Duisburg-Essen, Institute for Materials Science and CENIDE, Germany
3. University of Duisburg-Essen, Institute of Technology for Nanostructures, Germany

Perovskites have yielded a multitude of functionalities discovered over the last seventy years spanning from magnetism, ferroelectricity to supraconductivity. The most recent developments have brought forward hybrid halide perovskites containing a halide ion and a small organic molecule as constituents of the crystal structure. One of the most remarkable properties of these emergent materials is their high charge carrier mobility and an outstanding robustness of the electronic properties towards lattice defects. In this presentation the role of dielectric effects in this context will be outlined. Paraelectric effects will be contrasted to the role of apparent ferroelectricity and the potential misinterpretation of a number of experiments in this context.

5:15 PM

(EMA-060-2022) Effects of Ion Irradiation on Amorphous and Anatase TiO_2 Nanotube Anodes for Lithium-ion Batteries

T. Olsen*[1]; K. A. Smith[4]; A. I. Savva[7]; P. Barnes[1]; D. A. Tenne[1]; Y. Wang[6]; C. Yang[5]; K. Hattar[2]; J. Wharry[5]; H. Xiong[3]

1. Boise State University, USA
2. Sandia National Laboratories, USA
3. Boise State University, Materials Science and Engineering, USA
4. National Institute of Standards and Technology (NIST), USA
5. Purdue University, USA
6. Los Alamos National Lab, USA
7. Clean Energy Associates (CEA), USA

Recent studies have shown that electrochemical charge storage capacity of lithium-ion batteries can be enhanced by the presence of structural defects such as vacancies and interstitials. Here, we present on our recent work that demonstrates how ion irradiation can be used to intentionally create defects in anodically grown TiO_2 nanotubes, and corresponding changes in their electrochemical properties. We found that proton irradiation of both anatase and amorphous TiO_2 nanotube anodes improved the capacity and rate capability compared to unirradiated controls. This improvement was attributed to an increase in Li^+ storage sites and increased Li^+ diffusivity due to irradiation induced defects. An irradiation induced amorphous-to-crystalline transformation in amorphous TiO_2 nanotubes was also observed. We have been recently exploring how irradiation of TiO_2 nanotubes with ion species other than protons - such as Kr and Nb ions - change the morphology, electrical properties, and electrochemical properties of TiO_2 nanotubes. Irradiation by either Kr or Nb ions has been found to result in significant morphological changes to nanotubes.

S4: Complex Oxide Thin Films and Heterostructures: From Synthesis to Strain/ Interface-engineered Emergent Properties

Phenomena arising from Strain Couplings and Interface Couplings

Room: Orange A

Session Chair: Judith MacManus-Driscoll, University of Cambridge

10:00 AM

(EMA-016-2022) Embracing gradients (Invited)

G. Catalan*[1]

1. ICREA and ICN2, Spain

Strain is often used to change the properties of oxide thin films. It comes at a price, however: as film thickness increases, relaxation appears, causing the films' properties to change. Strain relaxation is therefore a problem for strain engineering. However, it also has a sunny side: it brings along emergent functionalities. One is of course flexoelectricity --a coupling between strain gradient and polarization that is allowed in all materials and can be large at the nanoscale. Another is ferroelastic domain formation, with the attendant properties brought on by domain walls. And gradients (of thickness, temperature, or strain) can also stabilize phase boundaries between different phases of the same material, so that different properties can be symultaneously displayed by the same sample (this is sometimes

called "Janus effect"). In antiferroelectrics such as PbZrO3, for example, one can have two sides of the same sample showing simultaneous positive and negative electrocaloric effects. In addition, strain-relaxing defects can themselves be interesting and useful. For example, in VO2, a material with a metal-insulator transition, strain relaxation happens through self-arranged crack patterns that physically separate individual tiles of single-crystalline film; this tiling behaves de facto as a self-patterned pixel array. In my talk, I will describe the above and some other ways in which we are taking advantage of gradients to generate new functionalities.

10:45 AM

(EMA-017-2022) Emergent Energy Conversion Effects at Symmetry-Engineered Heterostructures (Invited)

M. Yang*[1]; M. Alexe[1]

1. University of Warwick, Department of Physics, United Kingdom

Energy transduction has been an intensively and extensively studied topic for decades, due to its fundamental interests and technological importance. Just like any other physical effect, symmetry plays an essential role in energy transduction. For instance, only the materials without inversion symmetry possess the piezoelectric effect that converts mechanical energy to electricity and vice versa; materials with polar symmetry possess the pyroelectric effect that generates electricity once sensing a temperature variation. Here, we would like to introduce two emergent energy conversion effects at heterostructures induced by symmetry engineering, i.e., the interface piezoelectric effect and interface pyroelectric effect. The built-in electric field manifesting at the heterostructure interfaces, such as Schottky junctions, induces interface polar symmetry, giving rise to piezoelectric and pyroelectric effects, even though the component materials are centrosymmetric. These effects function in materials of any symmetry ranging from oxides, silicon, two-dimensional layered materials and even amorphous semiconductors, etc. More importantly, they exhibit coefficients comparable and even larger than conventional bulk materials, demonstrating their potentials in technological applications.

11:15 AM

(EMA-018-2022) Topological Hall effect like signatures in epitaxial oxide hetero-interface

P. Roy*[1]; A. Chen[2]; Q. Jia[3]

1. University at Buffalo-The State University of New York, Materials Design and Innovation, USA
2. Los Alamos National Lab, USA
3. University at Buffalo, Materials Design and Innovation, USA

In the past few years non-collinear or non-coplanar spin textures such as helices, domain walls, skyrmions etc. due to Dzyaloshinski-Moriya interaction in presence of broken inversion symmetry and strong spin orbit coupling have drawn a great amount of interest. Such spin textures can have promising applications in next generation nonvolatile memories, energy efficient nanoelectronics and spintronic devices. $SrRuO_3$ (SRO) is a 4d ferromagnet with multiple Weyl nodes at the Fermi level is one of the rare oxide where stable magnetic skyrmions and chiral magnetic domains are possible. Previously ferroelectric proximity and high spin-orbit coupling due to Ir at the hetero-interface have been found as an effective way to stabilize skyrmions in SRO thin films. Here we have investigated the magneto-transport property of SRO (ferromagnet) and $La_{0.48}Ca_{0.52}MnO_3$ (antiferromagnet) epitaxial hetero-interface and found that the strong interaction between these two oxides can exhibit topological Hall effect (THE) like signatures over a wide range of temperatures depending on the thickness of SRO, while the $La_{0.48}Ca_{0.52}MnO_3$ thickness remain fixed. The maximum THE was observed for 5 nm SRO film at 10K and the feature was present up to 80K. Our results suggest that competition between ferromagnetism and anti-ferromagnetism can also be a strategy to induce chiral spin structures in the ferromagnetic matrix of SRO.

11:30 AM

(EMA-019-2022) Piezoresponse and Schottky Currents Throughout Distinct Superlattice Layers via Tomographic AFM

T. J. Moran[1]; J. SONG[1]; K. Suzuki[2]; T. Hosokura[2]; R. Ramesh[3]; B. Huey*[1]

1. University of Connecticut, Materials Science and Engineering, USA
2. Murata Manufacturing Co., Ltd., R&D Center for Technology, Japan
3. UCBerkeley, MSE/Physics, USA

Functional properties throughout ferroelectric thin films and superlattices are of increasing importance as device dimensions continue to decrease for real world applications. In addition to thickness dependencies, demonstrated for monolithic films and with heterostructures, emergent phenomena may become detectible as lateral and normal dimensions shrink to few-nm or even unit cell length scales. This includes stable domain patterns, polarization magnitudes, ferroelectric hysteresis loops, and dielectric properties. Leveraging nanopatterning as well as Tomographic AFM, results are presented for $BaTiO_3$:$SrTiO_3$ and also $PbTiO_3$:$SrTiO_3$ superlattices with the aim of guiding future multilayer device designs.

In-situ Thin Film Characterization

Room: Orange A

Session Chair: James Rondinelli, Northwestern University

2:00 PM

(EMA-061-2022) Two-dimensional superconductivity at $KTaO_3$ interfaces (Invited)

A. Bhattacharya*[1]

1. Argonne National Laboratory, Materials Science Division, USA

In this talk, I will outline our discovery of superconductivity in electron gases formed at interfaces between (111) oriented $KTaO_3$ and insulating overlayers of either EuO or $LaAlO_3$. $KTaO_3$ is an incipient ferroelectric, a cousin of the more widely studied $SrTiO_3$, but with much higher spin-orbit coupling arising from the 5d states in Ta. In the $KTaO_3$ (111) interfacial superconductor, the value of T_c can be as high as 2.2 K, about one order of magnitude higher than in the $LaAlO_3$/$SrTiO_3$ system. Critical field and current-voltage measurements indicate that the superconductivity is two-dimensional. Using transmission electron microscopy and resonant x-ray scattering, we establish the presence of substitutional defects and vacancies at the KTO interface that can act as donors of electrons, and may lead to the formation of the interfacial electron gas. This interfacial superconductor has a number of unusual properties, including a strong orientation selectivity, and a large in-plane anisotropy in transport properties at low temperatures prior to the onset of superconductivity, where the nominally six-fold symmetry of the KTO (111) surface is spontaneously broken. I will briefly review recent developments in this field, and also point towards possible future directions.

2:45 PM

(EMA-062-2022) Performance loss of promising SOFC cathode materials by sub-ppm sulfur poisoning revealed by in-situ PLD and AP-XPS studies

C. Riedl*[1]; M. Siebenhofer[1]; A. Nenning[1]; R. Christoph[1]; M. Kubicek[1]; A. Limbeck[1]; A. K. Opitz[1]; J. Fleig[1]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria

Accelerating the oxygen reduction kinetics taking place on the surface of solid oxide fuel cell (SOFC) cathodes is an important goal of current research. In this contribution, five different mixed conducting cathode materials ($La_{0.6}Sr_{0.4}CoO_{3-\delta}$, $La_{0.6}Sr_{0.4}FeO_{3-\delta}$, $SrTi_{0.3}Fe_{0.7}O_{3-\delta}$, $Pr_{0.1}Ce_{0.9}O_{2-\delta}$ and $La_{0.6}Sr_{0.4}Fe_{0.985}Pt_{0.015}O_{3-\delta}$) were grown as dense thin films by pulsed laser deposition (PLD) and characterized directly after growth via electrochemical impedance spectroscopy inside the PLD chamber (i-PLD). This technique enables quantification of the oxygen reduction kinetics on contaminant-free surfaces unaltered by any external degradation. Our

measurements reveal the true catalytic power of the electrode and polarization resistances up to two orders of magnitude lower than previously reported in literature were measured. (e.g. for LSC an ASR of 0.15 Ωcm^2 was found, while usually > 1 Ωcm^2 are measured (synthetic air, 600 °C)) Ambient pressure X-ray photoelectron spectroscopy (AP-XPS) together with simultaneous in-situ impedance measurements revealed the presence of SO_x contaminations on the electrode surface to be strongly correlated with a huge performance loss of the SOFC cathodes. Already trace amounts of SO_x of the order of ppb present in high purity gases (99.999 %) are extremely detrimental leading to significantly increased polarization resistances.

3:00 PM

(EMA-063-2022) Thermally Stable Au-$BaTiO_3$ Nanoscale Hybrid Metamaterial for High Temperature Plasmonic Applications

D. Zhang*[1]; Z. Qi[1]; J. Jian[1]; J. Huang[1]; X. Phuah[1]; X. Zhang[1]; H. Wang[2]

1. Purdue University, Materials Engineering, USA
2. Purdue University, School of Materials Engineeringn, USA

The thermal stability of Au-$BaTiO_3$ nanocomposite thin film as a hybrid metamaterial deposited by one-step pulsed laser deposition (PLD) has been investigated via both an ex situ annealing followed by TEM analysis and an in situ heating study in TEM. For the ex situ annealing study, the XRD analysis shows good crystallinity for both as-deposited and annealed films after being annealed at 600°C for different time periods (i.e. 1, 3, 6, and 30 hrs.). The optical measurements including transmittance/reflectance, ellipsometry and Raman spectroscopy, all demonstrate excellent optical properties of the hybrid metamaterial films by exhibiting the static localized surface plasmon resonance (LSPR) peak and hyperbolic dispersion in the visible to near-infrared regime. Both TEM results of the ex situ annealed samples and in situ heating in TEM reveal no obvious microstructure change after the extensive high temperature annealing and suggest high thermal stability of the Au-oxide hybrid materials and their future applications in high temperature plasmonic applications.

3:15 PM

(EMA-064-2022) Advanced analysis of reflection high energy electron diffraction data

K. Gliebe*[1]; A. Sehirlioglu[2]

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

In-situ reflection high energy electron diffraction (RHEED) videos contain a plethora of information about the crystal structure and growth characteristics of thin films. However, only a very small portion of this data is generally utilized. We compared three dimension reduction techniques - principal component analysis, kmeans clustering, and nonnegative matrix factorization (NMF) - for the interpretability of the full RHEED videos. Through this analysis, we discovered that there is a phase shift in the intensity oscillations of different diffraction spots within the same RHEED pattern. Since intensity oscillations are used to determine the completion of a layer during growth of thin films, this phase shift indicates a different level of layer completion based on the choice of diffraction spot. Using our understanding of incoherent scattering and the information from the dimension reduction techniques, we were able to explain this phenomenon and the details for different diffraction spots. Additionally, we determined that NMF was the most effective dimension reduction technique for the understanding of RHEED videos.

Controlled Synthesis of Lateral and Vertical Heteroepitaxial Thin Films and Nanocomposites I

Room: Orange A

Session Chair: Anand Bhattacharya, Argonne National Laboratory

4:00 PM

(EMA-065-2022) The Electronic Structure of Degenerately N-doped Ga_2O_3 Thin Films (Invited)

H. Zhang*[1]

1. Xiamen University, College of Chemistry and Chemical Engineering, China

Ga_2O_3 is emerging as a promising wide bandgap semiconductor for high-power electronics and solar-blind ultraviolet photodetector. It is highly desirable to dope it with controllable carrier concentrations for different purpose of applications. This talk reports the realization of degenerate doping of Ga_2O_3 with Si (SGO) thin films with carrier concentrations ranging from 5×10^{18} up to 2.6×10^{20} cm^{-3}. A record high conductivity of 2500 S/cm and mobility of 60 cm^2/V s was achieved. The SGO films show a high transparency over a wide spectrum from visible to deep UV. Hard x-ray photoelectron spectroscopy (HAXPES), optical spectroscopy and DFT calculations were also performed to elucidate insights on the optical and electronic structures. HAXPES at the valence band observed the widening of bandgap as a result of occupation of the conduction band (CB) and the shrinkage of bandgap associated with many-body interaction. Supplemented with DFT, we demonstrate that the bandgap shrinkage mainly result from the change of CB induced by mutual electrostatic-interaction. Because the Si energy level is sitting 3 eV above the CB bottom, there is little hybridization between Si orbital and Ga 4s derived CB, leaving the CB edge unperturbed and a small electron effective mass maintained though the doping level is high.

4:30 PM

(EMA-066-2022) Material characterization and contact resistivity of LaCoO3 grown by optimized DC magnetron sputtering

R. Bhattacharya*[1]

1. UCLA, Materials Science and Engineering, USA

Novel transition metal compounds that exhibit rapid, reversible changes in conductivity as a function of temperature (a.k.a Insulator to Metal Transition) offer high switching ratios suitable for electronic switches and high power thermal management. This work demonstrates the thin-film growth of wafer-scale magnetron sputtered LaCoO3, a transition metal perovskite with a large magnitude Co (III) two-stage spin-state transition to metallic state at 500K. We present firstly on the influence of growth temperature, composition, and substrate choice on grain size, topology and crystallinity as studied by atomic force microscopy and x-ray diffraction. Temperature-dependent resistivity for epitaxial versus polycrystalline films is evaluated by four-point probe method and correlated to the high temperature bandgap-collapse observed by near-IR optical absorption. Finally, we will briefly discuss the evaluation of various e-beam evaporated metals and annealing procedures via the transmission line measurement method to determine the most thermally stable and lowest contact resistivity materials to aid in integration of LCO into power devices.

4:45 PM

(EMA-067-2022) Stress release via crystal rotation in epitaxial crystallization of amorphous complex oxides in complex geometries

R. Liu*[1]; P. Zuo[1]; S. Marks[1]; D. Sri Gyan[1]; D. E. Savage[1]; T. Zhou[2]; Z. Cai[3]; M. Holt[2]; S. E. Babcock[1]; T. F. Kuech[4]; P. G. Evans[1]

1. University of Wisconsin-Madison, Department of Materials and Engineering, USA
2. Argonne National Lab, Center for Nanoscale Materials, USA
3. Argonne National Lab, Advanced Photon Source, USA
4. University of Wisconsin-Madison, Department of Chemical and Biological Engineering, USA

Crystallization from an amorphous precursor via solid phase epitaxy enables a wide range of opportunities in the formation of oxide materials in new geometries. Key challenges to achieve nanoscale control of epitaxial crystallization are 1) selecting the sites of the initial step of crystallization and simultaneously maintaining a low rate of homogeneous nucleation away from epitaxial interfaces, 2) understanding the microscopic mechanism that leads to crystallization at amorphous/crystal interface in nanoscale complex geometries. Silicon nitride patterns were patterned on the surface of $SrTiO_3$ (STO) 001 single-crystal substrates using optical lithography. Amorphous STO was deposited on the patterned substrates at room temperature and crystallized by heating to temperatures at which crystallization occurred from seeds and the rate of homogeneous nucleation remained low. The results indicated that amorphous STO selectively crystallized on STO seed and laterally crystallized for distances of microns over the silicon nitride patterns. Synchrotron x-ray nanobeam diffraction imaging illustrated that the crystals rotate their orientations due to the formation of defects during crystallization. Initial indications are that the defects form as a result of the stress arising from the density difference between the amorphous and crystalline films.

5:00 PM

(EMA-068-2022) Nanoscale freestanding Sr_2IrO_4 thin-films for flexible electronics

S. Shrestha*[1]; M. Coile[1]; M. Souri[1]; M. Zhu[2]; J. Kim[1]; R. Pandey[1]; J. Brill[1]; J. Hwang[2]; J. Kim[3]; A. Seo[1]

1. University of Kentucky, Physics and Astronomy, USA
2. Ohio State University, MATERIALS SCIENCE AND ENGINEEING, USA
3. Argonne National Lab, Advanced photon source, USA

We report the structural and optical properties of 24-nm thick freestanding layered iridate (Sr_2IrO_4) epitaxial thin films fabricated using a water-soluble $Sr_3Al_2O_6$ layer. The coherent lattice structure, phonon modes, two-magnon Raman scattering, and optical absorption spectra of the freestanding Sr_2IrO_4 nanomembrane are analogous to those of the layered iridate epitaxial thin films and single crystals. It is noteworthy that 3-unit-cell-thick $SrIrO_3$ interfacial layers alleviate the formation of antiphase boundaries at the interface between Sr_2IrO_4 and $Sr_3Al_2O_6$, resulting in structurally robust freestanding thin films. Our experimental results show that this freestanding thin-film approach of layered oxides can provide techniques for tuning or realizing unprecedented states beyond conventional thin-film methods, suggesting a pathway in achieving flexible two-dimensional layered oxides electronics.

S6: Emerging Semiconductors Materials and Interfaces

Advances in Thin Film Synthesis I

Room: Citrus B

Session Chairs: Rafael Jaramillo, Massachusetts Institute of Technology; Matthew Brahlek, Oak Ridge National Lab

10:00 AM

(EMA-020-2022) Defect seeded lateral epitaxy and exfoliation on graphene terminated surfaces (Invited)

J. Kawasaki*[1]

1. University of Wisconsin, USA

We exploit defects in a 2D barrier layer to drive the seeded lateral epitaxy of atomically smooth, exfoliatable, single-crystalline membranes. This growth mode offers many of the advantages of the recently discovered remote epitaxy, including novel strain relaxation pathways and the ability to exfoliate free-standing membranes, plus additional advantages of (1) tolerance for imperfect graphene/substrate interfaces and (2) the ability to engineer the growth by patterning the 2D graphene layer. We show that GaSb films grow on graphene-terminated GaSb (001) via a seeded lateral epitaxy mechanism, in which pinhole defects in the graphene serve as selective nucleation sites, followed by lateral epitaxy and coalescence into a continuous film. These defects are created by native oxide desorption from the substrate. Importantly, the small size of the pinholes permits exfoliation of a continuous, free-standing GaSb membrane. By combining molecular beam epitaxy with \textit{in-situ} electron diffraction and photoemission, plus \textit{ex-situ} atomic force microscopy and Raman spectroscopy, we track the graphene defect generation and GaSb growth evolution a few monolayers at a time. Our discovery provides a highly tunable method to engineer single-crystalline 3D materials on precisely tuned 2D barriers. This work was supported by NSF and DARPA.

10:30 AM

(EMA-021-2022) Self-regulated growth of candidate topological superconducting parkerite by molecular beam epitaxy

J. M. Lapano[1]; T. Smith*[1]; Y. Pai[1]; A. R. Mazza[1]; J. Zhang[1]; T. Isaacs-Smith[2]; P. Gemperline[2]; L. Zhang[3]; H. Li[1]; H. Lee[1]; G. Eres[1]; M. Yoon[1]; R. B. Comes[4]; T. Z. Ward[1]; B. Lawrie[1]; M. McGuire[1]; R. Moore[1]; C. T. Nelson[1]; A. May[1]; M. Brahlek[1]

1. Oak Ridge National Lab, USA
2. Auburn University, USA
3. University of Tennessee, USA
4. Auburn University, Dept. of Physics, USA

Ternary chalcogenides such as the parkerites and shandites are a broad class of materials exhibiting a rich diversity of transport and magnetic behavior as well as an array of topological phases including Weyl and Dirac nodes. However, they remain largely unexplored as high-quality epitaxial thin films. In this talk, I will discuss the self-regulated growth of thin films of the strong spin-orbit coupled superconductor $Pd_3Bi_2Se_2$ on $SrTiO_3$ by molecular beam epitaxy. Films are found to grow in a self-regulated fashion, where, in excess Se, the temperature and relative flux ratio of Pd to Bi controls the formation of $Pd_3Bi_2Se_2$ due to the combined volatility of Bi, Se, and Bi-Se bonded phases. The resulting films are shown to be of high structural quality, the stoichiometry is independent of the Pd:Bi and Se flux ratio and exhibit a superconducting transition temperature of 800 mK and critical field of 17.7 ± 0.5 mT, as probed by transport as well as magnetometry. Understanding and navigating the growth of the chemically and structurally diverse classes of ternary chalcogenides opens a vast space for discovering new phenomena as well as enabling new applications. This work was supported by the

U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division, and the National Quantum Information Science Research Centers.

10:45 AM

(EMA-022-2022) Topological Tuning in $NiTe_{2-x}Se_x$ alloys

P. Nguyen*[1]; H. Nguyen[2]; T. Trinh[2]; J. Kim[2]; J. Lee[1]

1. Pusan National University, Department of Physics, Republic of Korea
2. University of Ulsan, Department of Physics, Republic of Korea

The group-X transition-metal dichalcogenides (TMDs) MX_2 (M=Ni, Pd, Pt; X=Se, Te) recently have attracted considerable interest as topological semimetals hosting new types of low-energy quasiparticles such as type-I and type-II Dirac fermions. The significant feature of this material classification is the strong tilted 3D Dirac cone, where electron/hole–like pockets touch at the Dirac point along a certain momentum direction in the electronic band structure. The symmetry-protected band crossing of the $p_{x,y}$ and p_z derived states of chalcogen atoms, abiding by intralayer hopping, crystal field splitting, and spin-orbit interaction effects, which gives rise to the formation of type-II bulk Dirac point (BDP-II). Here, by performing density functional theory (DFT) calculations combined with scanning tunnelling microscopy (STM), we systematically study the electronic and topological properties of type-II Dirac semimetal $NiTe_2$ via alloying with metastable $NiSe_2$. We find that alloying breaks electron-hole symmetry and then strongly modulate the electronic and topological properties of type-II Dirac semimetal $NiTe_2$. In this presentation, the underlying mechanism related to the topological tuning in $NiTe_{2-x}Se_x$ alloys will be discussed in detail.

11:00 AM

(EMA-023-2022) van der Waals Epitaxy on Freestanding Monolayer Graphene Membranes

J. M. Lapano[1]; O. Dyck[1]; A. R. Lupini[1]; W. Ko[1]; H. Li[1]; H. Miao[1]; H. Lee[1]; A. Li[1]; M. Brahlek[1]; S. Jesse[1]; R. Moore*[1]

1. Oak Ridge National Laboratory, USA

Due to unique structural and electronic properties that span the monolayer to bulk limits, two-dimensional (2D) and layered materials exhibit a wide range of properties that can enable new applications including optoelectronic functionalities and exotic topological phases of matter. Critical challenges center on controlling the atomic structure, understanding and controlling defects, and their incompatibility with existing semiconductor and nanofabrication techniques. In this talk I will introduce a new transformative materials approach where high-quality van der Waals epitaxial growth and characterization of layered 2D chalcogenide materials and heterojunctions are directly performed on freestanding monolayer graphene by molecular beam epitaxy. This "templated" synthesis approach is ideal for addressing the critical challenges in these materials, by, for example, enabling direct interrogation of the interfacial atomic structure of as-grown materials, and enabling designer interfaces to be created out of otherwise unstable materials combinations. This work opens routes toward creating new materials paradigms, better understanding the current generation of materials, as well as enabling the creation of device structures with more traditional semiconductor nanofabrication techniques.

11:15 AM

(EMA-024-2022) MBE Growth, Defect and Electronic Transport in Alkaline Earth Stannates (Invited)

B. Jalan*[1]

1. University of Minnesota, USA

Perovskite oxides have been the subject of intense ongoing study due to the diverse assortment of available properties and phenomena that they and their derivatives exhibit. However, until recently, there has been an unfilled gap for perovskite oxides that exhibit a high carrier mobility at room temperature. This gap was filled with the discovery of $BaSnO_3$ single crystals exhibiting room-temperature electron mobilities as high as 320 $cm^2V^{-1}s^{-1}$. Here we present the growth of epitaxial thin-films of $BaSnO_3$ and its noncubic analogs through the A-site substitution of Ba with smaller Sr and Ca. This includes a systematic doping study of $SrSnO_3$ over a wide range of carrier concentrations with record room-temperature electron mobilities exceeding 70 $cm^2V^{-1}s^{-1}$, and the first ever growth of $CaSnO_3$ by molecular beam epitaxy, whose ultrawide bandgap make it an encouraging ultra-wide bandgap material for applications in high-power devices and novel heterostructure-based transistors combining other functional perovskite oxides.

11:45 AM

(EMA-025-2022) Sputter Deposition of InN Thin Films for IR Plasmonic Applications

J. Nordlander*[1]; A. Cleri[1]; J. Hayden[1]; E. Runnerstrom[2]; J. Maria[1]

1. Penn-State University, USA
2. US Army Research Laboratory, USA

In this presentation, we demonstrate that reactive High-Power Impulse Magnetron Sputtering (HiPIMS) is an effective alternative for depositing high quality, epitaxial InN thin films on sapphire substrates. 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 while maintaining high electron mobilities in the deposited material. This unique capability set enables us to prepare high crystal quality epitaxial InN thin films with out-of-plane rocking curves of 0.1° or less and electron mobilities in excess of 400 cm^2/Vs. These thin films may be used as a material host for tunable IR light-matter interactions and the presentation will discuss the influence of deposition parameters on microstructure, electronic transport, and IR optical properties.

12:00 PM

(EMA-026-2022) In-situ investigation of the interface formation of Si-terminated diamond and a Nb_2O_5 electron acceptor layer for electronic applications

G. Abad*[1]; S. McDonnell[1]

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

Diamond, an ultra-wide bandgap semiconductor, has shown promise in high power, frequency, and temperature electronics; yet, issues with impurity doping has limited its use. Instead surface transfer doping has been used to induce a 2D hole gas at the diamond surface achieved by H-terminating diamond prior to the addition of an electron acceptor layer. Alternatively, we explore the combination of Si-terminated diamond and a Nb_2O_5 electron acceptor layer. Si will be electron beam deposited in ultra-high vacuum (UHV) onto diamond substrates then annealed to produce the (3x1) surface reconstruction reported for Si-terminated (100) diamond surface. In-situ characterization techniques including low energy electron diffraction (LEED), x-ray and ultraviolet photoelectron spectroscopies (XPS, UPS) will be used to confirm surface structure, analyze chemical composition, and measure work function, respectively. From these techniques, the degree of band bending and surface electron affinity will be determined. Nb will be deposited in an O_2 partial pressure to form the Nb_2O_5 electron acceptor layer. Aforementioned methods will be used to observe how interface chemistry, electronic structure, and band alignment evolve with Nb_2O_5 thickness. This work will culminate in a thermal stability study of the Nb_2O_5/Si-terminated diamond interface via UHV annealing.

12:15 PM

(EMA-027-2022) Novel Stabilization Mechanism on Polar Oxide Surface

J. Byun*[1]; Z. Wang[2]; S. Oh[2]; J. Lee[1]

1. Pusan National University, Department of Physics, Republic of Korea
2. SungKyunKwan University, Department of Energy Science, Republic of Korea

The stability of polar oxide surfaces has long been an interesting topic in surface science. Since the electrostatic potential diverges with increasing polar oxide thickness, various screening processes involve such as surface reconstruction, charge transfer, and adsorption of foreign charged species. Here, combining the density functional theory calculations and molecular dynamic simulations, we report that the vicinal surface steps can completely stabilize the polar oxide surface without introducing defects and excess charge. The evolution of steps at the vicinal surface, and resulting stabilized polar surface will be discussed and associated underlying mechanism will be introduced along with atomic-scale scanning transmission electron microscopy images.

Advances in Thin Film Synthesis II

Room: Citrus B

Session Chairs: Jason Kawasaki, University of Wisconsin; Rohan Mishra, Washington University in St. Louis

2:00 PM

(EMA-069-2022) Making Chalcogenide Perovskite Semiconductor Thin Films on Oxide Perovskite Substrates by Gas-Source Molecular Beam Epitaxy (Invited)

R. Jaramillo*[1]

1. Massachusetts Institute of Technology, USA

We demonstrate making $BaZrS_3$ thin films by gas-source molecular beam epitaxy (MBE). $BaZrS_3$ forms in the perovskite structure with corner-sharing ZrS_6 octahedra. The single-step MBE process makes films smooth on the atomic scale, with near-perfect stoichiometry and an atomically-sharp interface with the $LaAlO_3$ substrate. The films grow epitaxially via two, competing growth modes: buffered epitaxy, with a self-assembled interface layer, and direct epitaxy, with rotated-cube-on-cube growth. The films have a direct band gap, strong optical absorption, slow excited-state recombination (i.e., long minority carrier lifetime), and high charge transport mobility. This work sets the stage for developing chalcogenide perovskites as a family of high-performance semiconductor alloys with properties that can be tuned with strain and composition in high-quality epitaxial thin films, as has been long-established for other systems including Si-Ge, III-Vs, and II-Vs. The methods demonstrated here also represent a revival of gas-source chalcogenide MBE.

2:30 PM

(EMA-070-2022) Phase stability and optical property of quasi-one-dimensional $BaTiS_3$

G. Ren*[1]; B. Zhao[2]; A. Thind[1]; T. Cao[1]; J. Cavin[4]; J. Ravichandran[2]; R. Mishra[3]

1. Washington University in St.Louis, Institute of Materials Science and Engineering, USA
2. University of Southern California, Chemical Engineering and Material Science, USA
3. Washington University in St. Louis, Mechanical Engineering & Materials Science, USA
4. Washington University in St. Louis, Department of Physics, USA

$BaTiS_3$ has a quasi-one-dimensional structure with face-sharing (TiS_6) octahedral chains, and shows giant optical anisotropy. However, the crystal structure of $BaTiS_3$ has not been unambiguously determined from experimental measurements. Recent neutron scattering and single crystal X-ray diffraction studies show large atomic displacement parameters with anomalous temperature dependence raising the possibility of a lower symmetry compared to past structure refinement. To determine the most likely candidate structures, we performed density functional theory calculations in combination with group theoretical analysis to screen out three local energy minima with space groups of $P6_3cm$, $Cmc2_1$, and $P2_1$. Our phonon calculations identify soft-phonon-driven symmetry-lowering transitions for $Cmc2_1$ and $P2_1$ from $P6_3cm$ by involving in-plane displacements of Ti atoms. We further show the effect of these Ti displacements on the electronic and optical properties. Our theoretical calculations indicate that subtle changes in Ti displacements can lead to large birefringence and dichroism. This work establishes guidelines for tuning the linear optical properties of $BaTiS_3$ by changing the amplitude of Ti in-plane displacements.

2:45 PM

(EMA-071-2022) Optically Probing Quantum Spin Liquid Candidates and Toward Quantum Enhanced Optical Sensing (Invited)

Y. Pai*[1]

1. Oak Ridge National Lab, Materials Science and Technology Div., USA

CsYbSe$_2$, a recently identified quantum spin liquid (QSL) candidate, exhibits strong crystal electric field (CEF) excitations. Here, we identify phonon and CEF modes with Raman spectroscopy and observe strong CEF-phonon mixing resulting in a vibronic bound state. Complex, mesoscale interplay between phonon modes and CEF modes is observed in real space, and an unexpected nearly resonant condition is satisfied, yielding up to fifth-order combination modes, with a total of 17 modes identified in the spectra. This study paves the way to coherent control of possible QSL ground states with optically accessible CEF-phonon manifolds and mesoscale engineering of CEF-phonon interactions. On the other hand, we theoretically propose a truncated nonlinear interferometric readout for low-temperature magneto-optical effect measurements that is accessible with today's quantum optical resources. This research was sponsored by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Quantum Science Center, and by the Intelligence Community Postdoctoral Research Fellowship Program.

3:15 PM

(EMA-072-2022) Genetic Algorithm Structure Search for Epitaxial Growth Conditions of Cs-Sb Photocathodes on SiC(100)

J. Gibson*[1]; R. G. Hennig[1]

1. University of Florida, Material Science and Engineering, USA

Electron beams are an essential component in the development of a deeper understanding of quantum matter. The beam's spatial and temporal resolution depends directly on its brightness, which is controlled by the photocathode material. Binary compounds found in the Cs-Sb family grown on a SiC substrate have been identified as a potential photocathode material that can improve beam brightness. In this study, we utilize a genetic algorithm to search the potential energy surface to identify stable monolayers of Cs-Sb epitaxially grown on a SiC(100) substrate. Then, density functional theory is utilized to predict the material's photoemission properties. Finally, we calculate the surface free energy of the predicted surface structures over a range of chemical potentials and identify the most energetically favorable structure for the given chemical potential set. To aid experimental growth efforts for the epitaxial Cs-Sb layers, we convert the information into a surface phase diagram showing the structural stability as a function of the partial pressures of Cs and Sb during synthesis. All data produced in this study will be available on our open-source database MaterialsWeb.org.

4:00 PM

(EMA-073-2022) Graphene probe for the electrical properties at oxide film and graphene interfaces (Invited)

H. KANG*[1]

1. Pusan National University, Department of Physics, Republic of Korea

Graphene is well known to have the two dimensional hexagonal lattice structure and the linear dispersion relation, which lead many interesting phenomena. Among them, we have focused on two features to probe the properties of functional oxides; one is so called Dirac point (DP) where the conductance of graphene becomes minimum, and the other is half-integer quantum Hall effect (QHE). Dirac point was used to trace the change of thin film depending to the conditions, such as electric field or temperature. The universal quantized value in QHE gives us the quantitative information like dielectric constant. To explore the electrical properties of a high-k dielectric thin film and a ferroelectric material, the field-effect transistor type device was fabricated using functional oxides as gate dielectrics. We can elucidate the oxygen vacancy mechanism depending on the electric field and the complicated interface between ferroelectric and graphene with the two unique properties of graphene.

4:30 PM

(EMA-074-2022) "Atomic-level semiconductor" via flat phonon bands (Invited)

J. Lee*[1]

1. Ulsan National Institute of Science & Technology, Republic of Korea

We discovered that the elastic interaction between atoms in a solid completely disappears only when external voltage is applied in a compound with flat bands in polar phonon. Strikingly then each atom can be individually manipulated by voltage for information storage. This discovery will lead us to the design of ultimate-density memories. Just as Einstein's theory of relativity (E=mc2) enabled us to make bombs out of atoms, not out of matter, with our "Atomic Semiconductor" theory, we will open the era of making memories in an atomic scale rather than in materials scale. This theory is surprisingly applicable to the commercial ferroelectric HfO2 and thus can be realized in all electronic devices. Our paradigm shift will open the era of storing big data in the palm of your hand as the memory density will increase up to ~100 TB in the future according to the prediction of our theory.

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

New Superconductors, Unconventional Superconductors and Related Materials I

Room: Orange B

Session Chair: Michael Susner, The Air Force Research Laboratory

10:00 AM

(EMA-028-2022) Study of various superconductors grown at the National Cheng Kung University in Taiwan (Invited)

C. N. Kuo[1]; C. Lue*[1]

1. National Cheng Kung University, Department of Physics, Taiwan

In this talk, I will introduce various superconductors grown at the National Cheng Kung University in Taiwan. They include the two-dimensional structure superconductor $PdTe_2$, layered superconductor $AuSn_4$, cage structure superconductor $Lu_5Rh_6Sn_{18}$, and endohedral cluster superconductor Mo_8Ga_{41}. The single crystal synthesis and the superconducting properties of these materials will be presented. The prospective on the related superconductors will be discussed.

10:30 AM

(EMA-029-2022) Unconventional charge order and superconductivity in kagome materials (Invited)

J. Yin*[1]

1. Princeton University, USA

Lattice geometry, topological electron behaviour and the competition between different possible ground states all have a role in determining the properties of materials with a kagome lattice structure. In particular, the compounds KV3Sb5, CsV3Sb5 and RbV3Sb5 all feature a kagome net of vanadium atoms. These materials have recently been shown to exhibit superconductivity at low temperature and an unusual charge order at high temperature, revealing a connection to the underlying topological nature of the band structure. I will highlight these discoveries, place them in the context of the wider research effort in topological physics and superconductivity, and discuss the open problems for this field.

11:00 AM

(EMA-030-2022) Superconductivity in Europium Bismuth Sulfofluorides (Invited)

H. ZHAI*[1]

1. Northwest University, physics, China

The layered bismuth sulfofluorides $EuBiS_2F$ and $Eu_3Bi_2S_4F_4$ show unique properties among all the BiS_2-based superconductors. Both compounds exhibit a possible charge-density-wave (CDW) instability around 280 K and undergo superconducting transitions at 0.3 and 1.5 K, respectively, without extrinsic doping. The self-doping effect due to the mixed-valence state of Eu ions, which allows charge transfer from Eu to BiS_2 layers, accounts for the metallic behavior and superconductivity. Here we present a brief review of the research progress in these Eu-containing bismuth sulfofluorides, including the structure and electronic properties, external pressure effects, chemical pressure effects, and doping effects. The results can provide important information towards a deeper understanding of BiS_2-based superconductors.

11:30 AM

(EMA-031-2022) Where Will the Next Class of High-Temperature Superconductor Be Found? (Invited)

D. Parker*[1]

1. Oak Ridge National Lab, MSTD, USA

With the iron-based superconductors now of less interest comes a realization that a multiplicity of high-temperature superconductors have come into being, beginning with the cuprates, progressing to the unexpected, though rather conventional MgB_2, the extremely surprising iron-based materials, and the hydrides under high pressure, which display critical temperatures approaching room temperature. While each of these discoveries is remarkable in its own right, together they signal an age in which properties thought impossible now appear quite commonplace. At the same time, it is worth considering where the "next big discovery" might be made, particularly as regards superconductivity near (antiferro)magnetism, which is evident in the cuprates and iron-based materials. Is it the case that only electronic 3d shells greater than half-full are likely to yield a productive (i.e. $T_c > 10$ K) superconductivity? Or, as seems more likely, are there in fact numerous superconductors awaiting discovery from earlier transition metals such as Chromium? Which materials classes would be most likely for such a discovery? These issues will be discussed.

12:00 PM

(EMA-032-2022) Tomonaga-Luttinger liquid and superconductivity in quasi-one-dimensional $A_2Mo_3As_3$ metal (Invited)

D. Arcon*[1]; Z. Gosar[1]; B. Lv[2]

1. Institute Jozef Stefan, Condensed matter physics department, Slovenia
2. University of Texas, Dallas, USA

A universal paradigm of the Tomonaga-Luttinger liquid (TLL) describes the physics of interacting fermions in one dimension (1D) remarkably well and predicts their most characteristic features that can be directly verified in experiments: collective excitations which generally separate into spin and charge modes and a power-law decay of the correlation functions at long distances that lead to power-law dependencies of the corresponding experimental quantities as a function of temperature. While the vast majority of known physical realizations of TLL have repulsive interactions between collective excitation modes defined with the dimensionless interaction parameter $K < 1$, we here report that $A_2Mo_3As_3$ (A = K, Rb, Cs) is in the opposite and rarely investigated regime of attractive interactions. This is concluded from a characteristic power-law dependence of the alkali metal spin-lattice relaxation rates over a broad temperature range yielding the interaction parameter for charge modes $K > 1$. The TLL of the 1D band can be traced almost down to $T_c \approx 10.5$ K, where the bulk superconducting state is stabilized by the presence of a 3D band. The importance of structural instability of MoAs quasi-1D double-walled subnanotubes deduced from the ^{75}As NQR spectra together with the attractive interactions defining the precursor TLL are discussed in light of the unconventional superconducting state.

New Superconductors, Unconventional Superconductors and Related Materials II

Room: Orange B
Session Chair: Timothy Haugan, U.S. Air Force Research Laboratory

2:00 PM

(EMA-075-2022) Role of defects and magnetism on Ising superconductivity in monolayer $NbSe_2$ (Invited)

D. Wickramaratne*[1]

1. Naval Research Laboratory, USA

Monolayers of the superconducting transition metal dichalcogenides (TMD), eg. $NbSe_2$, exhibit a large anisotropy in the superconducting critical field. This phenomenon can be understood in terms of "Ising superconductivity" where the spins of the Cooper pairs are aligned perpendicular to the basal plane of the TMD. Doping Ising superconductors or forming vertical heterostructures of Ising superconductors with magnetic materials are of significant interest as they provide an opportunity to explore the interplay between proximity-induced magnetism, spin-orbit coupling and superconductivity. I will provide an overview of the physics of Ising superconductivity and how it is impacted by magnetism and point defects, using first-principles calculations and analytical theory. I will then discuss the ramifications of these effects using two case studies motivated by recent experiments. One is tunneling across 2D Ising superconductor/magnetic insulator heterostructures based on $NbSe_2$ and $CrBr_3$. Second, recent experiments have shown a non-monotonic change in the superconducting transition temperature in $NbSe_2$ alloyed with sulfur, which was interpreted as evidence of multifractal superconductivity. I will present an alternative explanation for the origin of this non-monotonic behavior of the transition temperature, that does not require the conjecture of multifractality.

2:30 PM

(EMA-076-2022) Pressure-induced high-temperature superconductivity retained at ambient pressure (Invited)

L. Deng*[1]; T. Bontke[1]; R. Dahal[1]; Y. Xie[3]; B. Gao[2]; X. Li[3]; K. Yin[4]; M. Gooch[1]; D. Rolston[1]; T. Chen[2]; Z. Wu[1]; Y. Ma[3]; P. Dai[2]; C. Chu[1]

1. University of Houston, Physics, USA
2. Rice University, Physics and Astronomy, USA
3. Jilin University, Physics, China
4. Linyi University, Physics and Electronic Engineering, China

Pressure has played a crucial role in the development of superconducting material due to the simplicity of varying the basic parameter of inter-atomic distance in a compound without introducing complications associated with altering its chemistry. Applying pressure to a material can tune its carrier concentration, shift its Fermi level, and even reshape its Fermi surface topology. In the pursuit of room-temperature superconductivity, all record superconducting transition temperatures (T_cs) reported in the past few decades have been achieved under high pressure, from 164 K in the $HgBa_2Ca_2Cu_3O_{8+d}$ cuprate under 32 GPa in 1994 to above 200 K in the hydrides above 150 GPa since 2015. While the record T_cs fall into practical cryogenic regimes for applications, the high pressure required to attain these superconducting states renders them impractical for significant applications and for comprehensive scientific inquiry. I will discuss recent breakthroughs in the design, synthesis, and kinetic stabilization of revolutionary materials with high T_cs and other novel properties, with a particular focus on understanding kinetic stabilization routes to retaining these properties under ambient pressure. Our recent work on FeSe demonstrates a possible path to retain lattice and/or electronic structures with desirable properties after removing the extreme conditions initially required to attain these properties.

3:00 PM

(EMA-077-2022) New Verbeekite-type polymorphic phase, superconductivity, and rich phase diagram in the $PdSe_{2-x}Te_x$ system (Invited)

w. liu*[1]; R. Mehrdad[1]; x. wang[3]; s. Li[1]; H. Wu[1]; P. Koirala[2]; M. Van de Pu[1]; V. William Gerard Hubert[2]; B. Lv[2]

1. UNIVERSITY OF TEXAS AT DALLAS, Physics, USA
2. University of Texas, Dallas, USA
3. University of Houston, USA

Recently, two-dimensional (2D) materials, including transition metal dichalcogenides (TMDs) have received considerable attention due to their emergent physical properties, which in turn have the potential to revolutionize many fields in both fundamental science and technological applications. Here we report a combined experimental and theoretical study of the $PdSe_{2-x}Te_x$ system. With increasing Te fraction, structural evolutions, first from an orthorhombic phase (Pbca) to a monoclinic phase (C2/c) and then to a trigonal phase (P-3m1), are observed accompanied with clearly distinct electrical transport behavior. The new monoclinic phase (C2/c) belongs to the very rare Verbeekite polymorphism and is discovered within a narrow range of Te composition ($0.3 \leq x \leq 0.8$). Superconductivity with enhanced critical temperature is observed within a narrow range of Te content ($1.0 \leq x \leq 1.2$). For $x = 1$, PdSeTe shows type-II superconductivity with enhanced T_c (2.73 K) and a nonbulk superconductivity nature with a volume fraction of ≈ 20% estimated from magnetic and heat capacity measurements. The rich phase diagram, new polymorphic structure, and abnormally enhanced superconductivity could further stimulate interest to explore new types of polymorphs and investigate their transport and electronic properties in the family of transition metal dichalcogenides.

4:00 PM

(EMA-078-2022) Enhanced superconductivity in tailor-made quasi-one-dimensional superconductors (Invited)

R. W. Lortz*[1]

1. Hong Kong University of Science & Technology, Department of Physics, Hong Kong

Quasi-1D superconductors have van Hove singularities that can lead to a greatly enhanced density of states at the Fermi energy, which is an important prerequisite for a high-temperature superconductor. Moreover, the region affected by the surface of the 1D structure, where phonon softening has an additional positive effect, acquires a significant volume fraction. However, in a single nanowire, fluctuations become strong and prevent a phase-coherent superconducting state. When many nanowires are arranged in parallel to form dense arrays, the electronic properties in the individual nanowires remain within the 1D limit, while transverse Josephson coupling can suppress fluctuations and stabilize zero-resistance. We have tailored quasi-1D arrays of ultrathin, weakly coupled nanowires. For many of them, we found enhanced superconductivity with critical temperatures well above bulk values. For example, for arrays of 5 nm Pb we found that the critical field increased by a factor of 200 and the superconducting transition was 4 K above the bulk transition. We even succeeded in fabricating 4-Angstrom 'sub-nanowires' of elemental Ga and Al in the pores of $AlPO_4$-5 zeolite. In the bulk, the critical temperatures are below 1 K, but in nanostructured form they rise to 7.7 K and 3.7, respectively. A dense arrangement results in Josephson coupling, stabilizing a phase-coherent superconducting phase.

4:30 PM

(EMA-079-2022) Superconductivity in one direction: the field-free Josephson diode (Invited)

H. Wu[1]; M. Ali*[1]

1. Delft University of Technology, Quantum Nanoscience, Netherlands

The superconducting analog to the semiconducting diode, the Josephson diode, has long been sought, with multiple avenues to realization proposed by theorists. Exhibiting magnetic-field free, single directional superconductivity with Josephson coupling of the supercurrent across a tunnel barrier, it would serve as the building-block for next-generation superconducting circuit technology. Here we first we discuss the field dependent superconducting diode effect and then the recently discovered field-free Josephson diode, created using an inversion symmetry breaking heterostructure of NbSe2/Nb3Br8/NbSe2. We demonstrate, for the first time without magnetic field, the junction can be superconducting in one direction while normal in the opposite direction. Based on that, half-wave rectification of a square-wave excitation was achieved with low switching current density (2.2 x 10^2 A/cm^2), high rectification ratio (10^4), and high robustness (at least 10^4 cycles). We also demonstrate symmetric delta_Ic (the difference between positive and negative critical currents) behavior with field and the expected Fraunhofer current phase relation of a Josephson junction. This realization raises fundamental questions about the Josephson effect through a non-trivial insulator when breaking symmetry, and opens the door to ultralow power, high speed, superconducting circuits for logic and signal modulation.

5:00 PM

(EMA-080-2022) Superconductivity in Moire Materials (Invited)

C. Lau*[1]

1. The Ohio State University, Department of Physics, USA

Arguably the most exciting development in materials science over the past few years is the rise of moire materials, the tailoring of electronic, thermal, mechanical, optical and optoelectronic properties of two-dimensional (2D) materials and heterostructures, by taking advantage of the formation of moiré superlattice that arises from either lattice mismatch or a small twist angle between adjacent atomic layers. In 2018, the amazing discovery of superconductivity and insulating states in "magic angle" twisted bilayer graphene (tBLG) has led to a "gold rush" of moirétronics studies, as researchers dash to investigate, theoretically and experimentally, the electronic properties and underlying mechanisms of various moire materials. Starting from twisted bilayer graphene, these devices soon expand to include twisted double bilayer graphene, monolayer on bilayer graphene, twisted homo-bilayer or hetero-bilayer transition metal dichalcogenides (TMDs), and trilayer graphene aligned with hexagonal BN (hBN). Here I will review the results and development in superconductivity and other correlated phases in moire 2D materials.

S10: Point Defects and Transport in Ceramics

Point Defect Segregation to Dislocations, Surfaces, Grain Boundaries, and Interfaces

Room: Cypress B

Session Chair: Divine Kumah, North Carolina State University

10:00 AM

(EMA-033-2022) Field-assisted sintering of Ta doped TiO_2

T. Kadosh*[1]; C. Nicollet[1]; J. Yang[1]; B. Yildiz[2]; H. L. Tuller[3]

1. MIT, DMSE, USA
2. Massachusetts Institute of Technology, USA
3. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA

Electric-field-assisted sintering (FAS) shows promise as a fast, energy-saving alternative for ceramic processing. It also offers advantages in controlling microstructure and homogeneity and in mitigating loss of volatile materials during sintering. Yet, the operative mechanisms remain controversial, including Joule heating, high heating rates, enhanced ion migration and/or redistribution at electrodes. Previous studies, however, lack a systematic examination of the sintering process as functions of the ionic defect species and their respective diffusivities/mobilities. Our study is designed to address these limitations. We investigated the relative roles of Joule heating and field induced ion migration in FAS of the model system by controlling relevant aspects of the material's defect chemistry and transport characteristics. We selected the donor dopant Ta to fix the sample conductivity that governs Joule heating of the sample, while systematically varying the Ti ion diffusivity that governs mass transport during sintering by controlling the oxygen partial pressure in the gas phase. Field induced changes in defect formation and migration energies are modeled in addition to potential Joule heating as sources of the FAS process. Representative electrical and densification data are presented and analyzed to aid in isolating Joule heating and field induced ion migration contributions.

10:15 AM

(EMA-034-2022) Electrical Reliability of Lead Zirconate Titanate Piezoelectric Films (Invited)

S. Trolier-McKinstry*[1]

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

Failure of lead zirconate titanate under DC electric fields occurs by a coupled failure mode in donor-doped, acceptor-doped, and films with graded doping. Curiously, the median failure time of PZT films can be increased on doping with either donors or Mn as an acceptor. The lifetimes under DC fields are controlled by migration of oxygen vacancies, coupled with changes in the interface barrier heights for conduction in thin films. The defect chemistry of the film, including variations in this defect chemistry at interfaces strongly influences both the failure and the asymmetry of the failure as a function of

the electrical polarity. It is possible to combine high piezoelectric responses with high lifetimes under DC electric fields through use of graded doping schemes through the film depth.

10:45 AM

(EMA-035-2022) Investigating oxygen reduction pathways on pristine SOFC cathode surfaces by in-situ PLD impedance spectroscopy

M. Siebenhofer*[1]; C. Riedl[1]; A. Schmid[1]; A. K. Opitz[1]; J. Fleig[1]; M. Kubicek[1]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria

The oxygen exchange reaction (OER) is the essential reaction for a variety of applications in a wide range of technologies. The detailed mechanism, however, is complex and still not completely understood. A comprehensive understanding of its mechanics is thus crucial regarding the optimization of devices and materials. In this contribution, the OER rates on pristine surfaces of different SOFC cathode materials (LSC, LSF, Pt:LSF, STF, PCO and LSM) were investigated via in-situ impedance spectroscopy during pulsed laser deposition (i-PLD). Besides demonstrating the astonishing catalytic capabilities of these materials, it is possible to investigate the OER based on experiments on clean surfaces unaltered by environmental degradation. All materials except LSM exhibit polarization resistances with very similar $p(O_2)$- and T-dependencies, differing only in their absolute value. In combination with defect chemical calculations, these results clarify several aspects of the OER and refine the understanding of the role of different defects in the reaction. We found that a large part of the effective activation energy, which is observed in equilibrium measurements, originates in thermally activated charge carrier concentrations. In a new approach, electrode polarization was used to control these defect concentrations and to extract concentration amended activation energies.

11:00 AM

(EMA-036-2022) Investigation of point defect segregation to planar faults in functional oxide thin films by scanning transmission electron microscopy (Invited)

A. Kumar[1]; S. Ning[1]; K. Klyukin[1]; B. Yildiz[1]; C. Ross[1]; J. LeBeau*[1]

1. Massachusetts Institute of Technology, USA

The electronic and magnetic properties of thin film functional oxides can be modified not only by the presence of antisite defects and antiphase boundaries (APBs), but also the interactions between them. In this talk, we will discuss how state-of-the-art atomic resolution imaging and spectroscopy with scanning transmission electron microscopy can directly probe the formation of point defects at and near planar faults, even at low concentrations. Using the YFeO3 multiferroic thin film system as a case study, we will show that Y_Fe antisite defects form throughout the bulk of the material by using atomic resolution energy dispersive X-ray spectroscopy, and give rise to ferroelectric behavior. At the APBs, we will also show that significant relaxation occur, in conjunction with unusual Fe_Y antisite defects (not found in the bulk of the structure) which are periodically distributed at the boundary. From theory, we will show that the APBs are polar and bi-stable, a consequence of their local structural and chemical environment. Furthermore, the presence of the Fe_Y antisites will be shown to significantly decrease the switching barrier, and thus potential pinning sites. We will conclude with a discussion of how APBs can stabilize point defects that would otherwise not be expected to form within the structure.

Defect Mediated Properties

Room: Cypress B

Session Chair: Zhongming Fan, Pennsylvania State University

2:00 PM

(EMA-081-2022) Oxygen vacancy-induced anomalous Hall effect in KTaO3 (Invited)

A. Al-Tawhid[1]; j. kanter[3]; M. Hatefipour[3]; D. Irving[1]; D. P. Kumah[2]; j. shabani[3]; K. Ahadi*[1]

1. NCSU, USA
2. North Carolina State University, Physics, USA
3. New York University, USA

The anomalous Hall effect, a hallmark of broken time-reversal symmetry and spin-orbit coupling, is frequently observed in magnetically polarized systems. Its realization in non-magnetic systems, however, remains elusive. Here, we report on the observation of anomalous Hall effect in nominally non-magnetic $KTaO_3$. Anomalous Hall effect emerges in reduced $KTaO_3$ and shows an extrinsic to intrinsic crossover. A paramagnetic behavior is observed in reduced samples using first principles calculations and quantitative magnetometry. The observed anomalous Hall effect follows the oxygen vacancy-induced magnetization response, suggesting that the localized magnetic moments of the oxygen vacancies scatter conduction electrons asymmetrically and give rise to anomalous Hall effect. The anomalous Hall conductivity becomes insensitive to scattering rate in the low temperature limit (T<5K), implying that the Berry curvature of the electrons on the Fermi surface controls the anomalous Hall effect. Our observations describe a detailed picture of many-body interactions, triggering anomalous Hall effect in a non-magnetic system. https://arxiv.org/abs/2109.08073

2:30 PM

(EMA-082-2022) Intrinsic point defects in Sodium Niobate studied with hybrid density-functional theory.

L. Villa*[1]; E. Ghorbani[1]; K. Albe[2]

1. Technical University Darmstadt, Materialwissenschaft, Germany
2. Technical University Darmstadt, Fachgebiet Materialmodellierung, Germany

In recent years extended research has been focusing on improving the properties of capacitors for energy storage applications. In this context, lead-free antiferroelectric materials (AFE) are excellent candidates due to their ability of displaying high energy density, high energy efficiency and low environmental impact. In this class of compounds, $NaNbO_3$ is amongst the most promising materials, due to the possibility to obtain double P-E loops at room temperature. One of the mostly used methods to obtain narrower antiferroelectric P-E loops is via doping. When impurities are introduced into a system, they will interact with the already present intrinsic defects. This can have an impact on the role that dopands play in the stabilization of the AFE phase. In order to investigate the role of intrinsic defects, we have studied the contribution of vacancies and of complexes of vacancies to intrinsic electron and hole conductivity. All calculations were performed in the framework of Density Functional Theory using Hybrid functionals. In particular, we have investigated the formation energies of all vacancy types considering all possible charge states in different regions of the stability diagram.

2:45 PM

(EMA-083-2022) Kinetic and atomistic origin of oxygen bubble formation in SOEC electrolytes

Y. Dong*[1]; J. Li[1]

1. Massachusetts Institute of Technology, USA

High-current-density operations of solid oxide electrolysis cells (SOECs) often result in accelerated degradations, including electrolyte degradations in the form of grain-boundary oxygen bubble formation and eventually transverse cracking of electrolyte

membrane. Here we shall discuss the kinetic and atomistic origin of such oxygen bubble formation, focusing on additional effects beyond well-known electrode (anodic) overpotential. We proposed that the unexpected internal phase forms because of a large potential jump across the ion-blocking transverse grain boundaries (which is needed to maintain constant ion and electron flow). It correctly explains the selective grain-boundary orientation responsible for oxygen bubble formation and offers definite rules for damage predict and mitigate. First-principles calculations were then conducted to illustrate the atomistic model of hole states in oxidized zirconia electrolyte, for p-type conduction (electronic leakage) and oxygen bubble formation (damage).

3:00 PM

(EMA-084-2022) Tailoring Defect-Induced Strain in Oxide Perovskites (Invited)

N. H. Perry*[1]

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

The coupling between point defect concentration changes and strain in inorganic materials may engender mechanical failure in solid-state ionic devices (batteries, fuel/electrolysis cells), thus constraining their design and materials choice. Conversely, chemo-mechanical coupling benefits new strain-based methods for characterizing defect equilibria and kinetics as well as design of new (electro)chemical actuators for extreme conditions. Rational materials design for these applications requires an understanding of how to tailor the strain-defect relationship. The key metric of interest is the coefficient of chemical expansion (CCE), which normalizes the strain to the point defect concentration change. In this talk I will describe our recent experimental and computational work targeting design principles for tailored CCEs and demonstrate modification of the CCE by as much as 500% through their application. In situ X-ray diffraction, dilatometry, and thermogravimetric analysis of CCEs have been combined with density functional theory simulations of Pr-oxide perovskite mixed conductors undergoing redox as well as Zr/Ce-oxide perovskite proton conductors undergoing hydration. We demonstrate key roles of a) perovskite tolerance factor and b) anion states' proximity to the Fermi level for tailoring CCEs and thereby introduce near-zero-strain electrode and electrolyte candidates for stable high-temperature electrochemical devices.

4:00 PM

(EMA-085-2022) Electronic And Magnetic Coupling at Transition Metal Oxide Interfaces (Invited)

D. P. Kumah*[1]; X. Zhang[1]; A. Penn[2]

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

The ability to control and probe orbital, electronic and spin degrees of freedom in two-dimensional transition-metal oxides has led to the discovery and understanding of a wide range of condensed matter phenomena including metal-insulator transitions, and emergent magnetism. Progress in the field has been driven by advances in the atomic-scale synthesis of crystalline 2D multilayered systems, where strain and interfacial interactions can be systematically tuned to realize novel electronic and magnetic ground states. Additionally, the development of high-resolution synchrotron X-ray diffraction and spectroscopy techniques allows for non-destructive and in-operando probes of materials to elucidate structural and electronic changes at interfaces between dissimilar oxide films. To illustrate the intimate link between interface-driven atomic-scale distortions and the physical properties of low-dimensional systems, this talk will focus on understanding the role interfacial and surface reconstructions play in driving experimentally observed thickness-dependent metal-insulator and magnetic transitions in the 3d and 4d transition metal oxide systems. Guided by first-principles theory, the talk will highlight how atomic-scale materials growth techniques and state-of-the-art methods to characterize their physical properties at the picometer-scale, provide a powerful approach for discovering novel quantum materials.

4:30 PM

(EMA-086-2022) Influence of local charge and magnetic ordering on point defect properties in magnetite (Fe_3O_4)

S. Srivastava*[1]; B. P. Uberuaga[2]; M. Asta[1]

1. University of California Berkeley, Materials Science and Engineering, USA
2. Los Alamos National Laboratory, Materials Science and Technology Division, USA

The thermodynamics and kinetics of point defects plays an important role in the fabrication, operation and degradation of electroceramics based devices. In the complex oxides involving transition metal ions such as Fe, the strong coupling of charge and spin configurations of point defects with the bulk electronic and magnetic structure strongly influences the ionic transport processes in these materials. As part of an effort aimed at understanding such processes under conditions involving irradiation induced defect production, this work is focused on understanding the equilibrium and non-equilibrium properties of point defects in magnetite (Fe_3O_4). Specifically, we employ first-principles calculations to investigate formation and migration energies of point defects in this material. The low-temperature structure of magnetite features coupled charge, spin and orbital order. This phase undergoes an order-disorder phase transition at around 120K, but there is evidence of strong local order above this transition. A specific focus of the calculations is understanding the effect of this local order on the properties of vacancy and interstitial point defects. The implications of these results on the transport through iron oxide heterostructures grown on iron will be discussed.

4:45 PM

(EMA-087-2022) Structure and electrical conduction properties of grain boundaries and domain-walls in $LiNbO_3$ (Invited)

A. Nakamura*[1]

1. Osaka University, Department of Mechanical Science and Bioengineering, Japan

Lithium niobate ($LiNbO_3$) is widely used for various devices because of its excellent piezoelectric and electro-optic properties as a ferroelectric material. The physical properties of $LiNbO_3$ are strongly influenced by the boundaries between domains and grains. Therefore, it is essential to understand atomic structures of the boundaries and their functional properties. In this study, we fabricated $LiNbO_3$ bicrystals with specific domain-walls or grain boundaries between different domains or orientations by diffusion bonding, and then analyzed the atomic structures of the boundaries by using scanning transmisson electron microscopy (STEM). In addition, we evaluated the electrical conduction properties of the boundaries at room temperature by using scanning probe microscopy and a semiconductor parameter analyzer. The results show that the domain-walls and boundaries often exhibit unusual electrical conductivity due to localized point defects when they are subjected to heat treatment or electric fatigue.

S11: Evolution of Structure and Chemistry of Grain Boundaries and Their Networks as a Function of Material Processing

Interface Structure and Chemistry

Room: Magnolia B/C

Session Chair: James Wollmershauser, U.S. Naval Research Laboratory

10:00 AM

(EMA-037-2022) Impact of Aliovalent Alkaline-Earth Metal Solutes on Ceria Grain Boundaries (Invited)

A. Singh*[1]

1. Arizona State University, Physics, USA

Ceria is an excellent ion-transport and ion-exchange material when used in polycrystalline form and with a high concentration of aliovalent doped cations. Despite its widespread application, the impact of atomic-scale defects in this material is poorly understood. In this study, using first-principles simulations, we provide a fundamental understanding of the atomic-structure, thermodynamic, and electronic properties of undoped grain-boundaries (GBs) and alkaline-earth metal (AEM) doped GBs in ceria. Using density-functional theory simulations, with a GGA+U functional, we find the Σ3 (111)/[01] GB is energetically more stable than the Σ3 (121)/[01] GB due to the larger atomic coherency in the Σ3 (111)/[01] GB plane. We dope the GBs with ~20% $[M]_{GB}$ (M=Be, Mg, Ca, Sr, & Ba) and find that the GB energies have a parabolic dependence on the size of solutes, the interfacial strain, and the packing density of the GB. We see a stabilization of the GBs upon Ca, Sr, and Ba doping whereas Be and Mg render them energetically unstable. The electronic density of states reveal that no defect states are present in or above the bandgap of the AEM doped ceria, which is highly conducive to maintain low electronic mobility in this ionic conductor. This work advances the atomic-scale understanding of aliovalent cation doped ceria GBs serving as an anchor to future studies that can focus on improving ionic transport.

10:30 AM

(EMA-038-2022) Atomic Scale Defect Chemistry at Grain Boundaries using 4-D STEM and APT (Invited)

B. P. Gorman*[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA

Determining defect chemisty at grain boundaries requires an exceptional combination of spatial and chemical resolution. Atomic structure of small volumes can be measured using scanning transmission electron microscopy (STEM), however, STEM does not have the necessary sensitivity to determine defect chemistry. Atom probe tomography (APT) has the ability to measure the isotopic identity of individual atoms using mass spectrometry, however, the spatial resolution of APT is not well defined. Combining 4-D STEM with APT into a single measurement, point defect accumulation at grain boundaries can be determined in 3-D. Examples of these measurements will be illustrated for several different oxides. Doped alumina showed small variations in oxygen stoichiometry while undoped alumina showed no change at the analyzed grain boundaries. Doped ceria also showed oxygen sub-stoichiometry at grain boundaries, along with a change in cation valence as measured by electron energy loss spectrometry. Such measurements allow for quantitative correlation between the atomic structure and the grain boundary dominated ionic conductivity. Future studies will improve the spatial resolution of this technique to 5 pm, enabling correlation between experiment and first principles theory. As a result, direct correlations between experiment and grain boundary dominated properties (electrical, mechanical, and optical) may be achieved.

11:00 AM

(EMA-039-2022) Grain Boundary Segregation and Energy in Multiphase Oxide Ceramics Processed by Different Sintering Techniques (Invited)

W. Bowman*[1]; K. Syed[1]; M. Mecartney[1]

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

Grain boundary (GB) chemical segregation and energy has been widely studied for single-phase ceramic systems. Yet there is limited understanding of how various processing techniques affect these in multiphase ceramics. Here I discuss our recent work to understand GB segregation and energy in multiphase oxide ceramics processed by three sintering techniques (conventional, flash, and spark plasma), using STEM-EDS and AFM. The 3-phase ceramics comprise 8 mol% Y2O3 stabilized ZrO2, α-Al2O3 and MgAl2O4. We find that the type of segregation at any particular interface does not change with different sintering processes, but the quantity of segregants is directly affected by processing type. We find too that GB energies play a critical role in microstructural evolution in multiphase ceramics, and report that energies of heterointerfaces are intermediate between the GB energies of the constituent phases.

11:30 AM

(EMA-040-2022) Interaction of Ytterbium Pyrosilicate Environmental-Barrier-Coating Ceramics with Molten Calcia-Magnesia-Alumonosilicate Glass

H. Sternlicht*[1]; N. P. Padture[2]

1. National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, USA
2. Brown University, School of Engineering, USA

Environmental barrier coatings (EBCs) are used to protect SiC based 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-aluminosilicate (CMAS) particles from the atmosphere, which can lead to premature coatings failure. Ytterbium pyrosilicate (monoclinic crystal structure) is a promising system for EBC ceramics. Thus, in this work grain boundaries in spark plasma sintered (SPSed) ytterbium pyrosilicate were studied using electron microscopy, focusing on defects along the boundaries (disconnections) and grain boundary chemistry. These were also studied after the interaction with CMAS glass at 1500°C, looking for alterations resulting from the interaction with the glass. Finally, phase boundaries before and after the interaction with the glass were characterized and compared to the grain boundaries mentioned above. These findings were correlated to the microstructural trends detected in the SPSed pellets before and after the interaction with the glass.

11:45 AM

(EMA-041-2022) Thermal, electrical, and microstructural characterizations of copper-tungsten (Cu/W) multilayers grown under compressive and tensile stresses

M. Hoque*[1]; G. Lorenzin[2]; D. Ariosa[2]; J. Tomko[1]; C. Cancellieri[2]; P. E. Hopkins[3]

1. University of Virginia, Mechanical and Aerospace Engineering, USA
2. Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland
3. University of Virginia, Departments of Mechanical and Aerospace Eng./ Materials Science and Eng./Physics, USA

Copper-tungsten (Cu/W) multilayers are one of the most widely used nanomaterials in electronic, optical, and sensing devices. The growth stresses generated in these multilayers can adversely impact the heat dissipation rate, thereby affecting the device functionality and reliability. To study such effects, in this work, we investigate the influence of tensile and compressive stresses on the thermal

conductivity of Cu/W multilayers grown via magnetron sputtering. The tensile stress leads to a disordered, open-porous structure with significant intermixing between the Cu and W layers. The compressive multilayer, on the other hand, possesses a more stable, nonporous structure with almost no intermixing. Due to such microstructural differences, the thermal and electrical conductivities of the compressive sample are more than a factor of two higher than those of the tensile specimen. Additionally, the thermal and electrical conductivities of both types of multilayers change significantly with annealing temperatures. This follows the microstructural changes as high annealing temperature (800 ºC or higher) causes the multilayers to degrade and turn into nanocomposites. The findings of this study are highly relevant to the usage of Cu/W multilayers in interconnect systems.

Microstructure Evolution

Room: Magnolia B/C

Session Chair: James Wollmershauser, U.S. Naval Research Laboratory

2:00 PM

(EMA-088-2022) Fundamental Insights into Microstructure and Properties of Ceramics Densified with the Cold Sintering Process (Invited)

C. Randall*[1]; S. H. Bang[1]; A. Ndayishimiye[1]; Z. Grady[1]

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

The physical properties of a material are determined by the microstructure that evolves under processing. The nature of the properties is dominated by the grain boundary. In cold sintering, the densification is controlled through consecutive chemical reactions of dissolution, grain boundary transport, and precipitation into pore structures. In this talk, we will discuss the evidence of the grain boundary and microstructural development, and the transport process will be considered from the perspective of pressure solution creep in multiple types of electroceramics that have been successfully cold sintered. A mechanism that underpins pressure solution creep was first described by the geologist Sorby (1863), who discussed mechanical force enhanced chemical reactivity to explore pit formations in pebbles. The phenomenological rates that controls the densification and grain growth processes will be discussed with our kinetic data, and linked to the pressure assisted creep, at these low temperatures.

2:30 PM

(EMA-090-2022) Conductive hotspots in Hf0.5Zr0.5O2: an automated experiment investigation

Y. Liu*[1]; S. Fields[2]; K. P. Kelley[1]; S. Jesse[1]; S. Trolier-McKinstry[3]; M. Ziatdinov[1]; J. Ihlefeld[2]; S. Kalinin[1]

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

HfO_2-based materials exhibit robust ferroelectricity even at extremely thin thickness, leading to a wide range of applications in ferroelectric devices. However, the local uniformity and leakage current of HfO_2 materials have been rarely investigated, which are important for the device performance. Here, we developed an automated scanning probe microscopy workflow to study the local conductivity of a Hf0.5Zr0.5O2 (HZO) thin film, which enables discovering leakage spots and subsequently performing detailed studies of these spots automatically. This automated workflow maps a large field of view of material first and automatically locates the leakage spots; then, detailed zoom-in measurements are automatically performed in the spots to systematically understand the material under study. Further, we embedded a drift correction--a shift-invariant variational autoencoder framework--algorithm to solve the image drift problem during measurement. Finally, we investigated the heterogeneous conductivity of the HZO thin film using this automated SPM approach, revealing the evolution of conductive hotspots around several tens nanometers in HZO with bias voltage and time. The hotspots show complex spatiotemporal dynamics as a function of time and bias, suggesting the presence of complex conduction mechanisms. We believe that approach developed in this work will be universally useful for other microscopy measurements.

2:45 PM

(EMA-091-2022) Engineering Grain Boundary Anisotropy to Suppress Abnormal Grain Growth in Alumina

B. Conry*[3]; M. Kole[3]; J. Harley[1]; M. R. Tonks[3]; M. Kesler[2]; A. Krause[3]

1. University of Florida, Electrical and Computer Engineering, USA
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3. University of Florida, Materials Science and Engineering, USA

Grain growth is a critical mechanism to ceramics processing, as grain size plays a major role in bulk material properties. Abnormal grain growth (AGG) is a process by which a small fraction of grains grow faster than their neighbors, resulting in a bimodal grain size distribution and heterogeneous bulk properties. The cause and underlying mechanisms behind AGG are poorly understood, although it has been theorized that anisotropy of grain boundary energy is directly related to AGG. We employ magnetically-induced texturing of Ca-doped alumina, a widely used ceramic in industry that is known to exhibit significant grain boundary energy anisotropy, to investigate this theory. The strong texture encourages the formation of energetically favorable grain boundaries, resulting in a preferential, anisotropic grain boundary character distribution. We hypothesize that abnormal grain growth is suppressed in these textured materials due to the widespread development of these preferentially oriented grain boundary networks. We will discuss and compare the prevalence and propagation of energetically favorable grain boundaries between textured and non-textured Ca-doped alumina heat treated for different times at 1600 C. These results will then be correlated to abnormal grain growth nucleation and propagation to explore the possibility of controlling abnormal grain growth phenomena in alumina.

Processing Parameters

Room: Magnolia B/C

Session Chair: Amanda Krause, University of Florida

4:00 PM

(EMA-092-2022) Structure, Chemistry and Composition of Grain Boundary Complexions in Boron Suboxide (Invited)

K. D. Behler*[1]; C. J. Marvel[2]; J. LaSalvia[1]; J. Synowczynski-Dunn[1]; W. T. Shoulders[1]; S. Walck[3]; H. Payne[4]; T. W. Moore[3]; M. P. Harmer[2]

1. U.S. Army Research Laboratory, DEVCOM, USA
2. Lehigh University, USA
3. SURVICE Engineering, USA
4. CQL at DEVCOM ARL, USA

Boron suboxide (B_6O) is a promising armor ceramic due to its combination of low density and high hardness which arises from its crystal structure and atomic bonding. Unfortunately, these also contribute to its poor intrinsic fracture resistance. One strategy to improve fracture resistance is to modify grain boundary complexions such that the boundaries are weakened, thereby promoting fracture mechanisms such as crack deflection. Depending upon raw materials and processing additives, boron suboxide can exhibit several distinct complexions including monolayers and glassy nanolayers. The role ceramic processing was investigated through sintering aid composition, hot-pressing time and temperature. While the addition of up to 5% SiO_2 resulted in abnormal grain growth (AGG), co-doping with rare earth oxides resulted in either suppression or enhancement of AGG, bimodal microstructures and the formation of chemically

distinct disordered nanolayers. The resultant microstructures and complexions were determined using aberration-corrected scanning transmission electron microscopy (AC-STEM) in combination with x-ray energy dispersive spectroscopy (EDS) and ζ-factor microanalysis. The experimentally measured grain boundary compositions and structures of each complexion type were used as input parameters for first-principles density functional theory (DFT) calculations to verify they were in equilibrium.

4:30 PM

(EMA-093-2022) Effect of Reduced Atmosphere Sintering on Blocking Grain Boundaries in Rare-Earth Doped Ceria (Invited)

J. Nino*[1]

1. University of Florida, USA

Rare-earth doped ceria is one of the top choices for use in electrolytes and composite electrodes in intermediate temperature solid oxide fuel cells. Trivalent acceptor dopants such as gadolinium mediate the ionic conductivity in ceria by creating oxygen vacancies and have a tendency to segregate at grain boundaries and triple points. This leads to formation of ionically resistive blocking grain boundaries and necessitates high operating temperatures to overcome this barrier. In an effort to improve the grain boundary conductivity, we studied the effect of a modified sintering cycle, where 10 mol% gadolinia doped ceria was sintered under a reducing atmosphere and subsequently reoxidized. In this presentation, based on a detailed analysis of the complex impedance, conductivity, and activation energy values, we will show that the ionic conductivity improves when compared with conventionally processed samples sintered in air primarily due to a drop in the grain boundary resistance. Combined with our previous work on microstructural and chemical characterization, we will show that this drop can be attributed to a diminished blocking effect of defect-associates at the grain boundaries. Promisign procesing and composition approaches for the further enhancement of the ionic conductivity in these materials via grain boundary engineering will be discussed.

5:00 PM

(EMA-094-2022) Overcoming microstructural homogeneity in ceramic battery electrolytes sintered by flash and cold sintering

G. Jones[1]; D. Dabera[1]; P. Tabrizian[1]; C. Green[3]; S. Ghanizadeh[3]; S. Fisher John[3]; S. Gorman[2]; G. West[1]; D. Pearmain[3]; E. Kendrick[2]; C. E. Dancer*[1]

1. University of Warwick, Warwick Manufacturing Group, United Kingdom
2. University of Birmingham, School of Metallurgy and Materials, United Kingdom
3. Lucideon Ltd., United Kingdom

Low energy processes such as flash and cold sintering enable rapid densification of ceramic materials at reduced temperatures. They are particularly attractive for sintering volatile materials, such as oxide-based solid-state electrolytes, which for solid-state battery manufacturing at scale will require coprocessing with metals. However, low energy processes can result in significant microstructural heterogeneities causing variability in the electrochemical performance. Here we present an overview of these effects and how they may be overcome in sodium-beta" alumina and lithium lanthanum zirconium oxide (LLZO). During flash sintering we have used multielectrode and contactless electrode systems to increase homogeneity. In cold sintering we studied the effects of temperature, pressure, and additions on the microstructure. The resulting materials are compared by examination of the microstructural features of the sintered ceramics by techniques including scanning electron microscopy, X-ray diffraction, and Raman spectroscopy. Initial observations of the densified LLZO electrolyte morphology using a novel hybrid SEM-FIB-SIMS approach are also discussed. We observe the chemical distribution of lithium additive materials which form a 3D conductive path through the electrolyte material and improves the electrochemical performance compared to materials without additives.

5:15 PM

(EMA-095-2022) Electroceramics with functional grain boundaries via cold sintering

J. M. Garcia*[1]; S. Dursun[1]; K. Tsuji[1]; A. Ndayishimiye[1]; S. H. Bang[1]; Z. Fan[1]; B. M. Foley[1]; C. Randall[1]

1. Pennsylvania State University, USA

Grain boundary engineered electroceramics are commonly composites with a matrix of insulating or semiconducting polycrystalline ceramic materials where the properties are associated to how their constituent materials are arranged and processed. In this research project we investigate various electroceramic composites and analyze the nature of their properties with respect to the structure enabled by the Cold Sintering Process. Experimental results present the succesful integration of a ferroelectric phase as a functional grain boundary, including details of the dielectric relaxations and conduction mechanisms through a grain boundary and through a sequence of all the microstructure of a polycrystalline matrix of Zinc Oxide (ZnO) semiconductive ceramic with Poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) ferroelectric polymer system. Additional results include the processing, characterization and analysis of the structure-properties relationship for Disodium Dimolybdate ($Na_2Mo_2O_7$) with the integration of high thermal conductivity (κ) fillers between its grain boundaries, such as nano-Diamond particles, for high power and high frequency applications by the improvement of thermal conductivity and dielectric loss. The understanding of the local interfacial nature of the functionality of such grain boundaries will guide to future novel compositions designed with Cold Sintering.

5:30 PM

(EMA-096-2022) Processing and Properties of High Interfacial Structure Nanocomposite Ceramics

J. Wollmershauser*[1]; K. Anderson[2]; B. Greenberg[3]; H. Ryou[1]; E. Gorzkowski[1]; B. Feygelson[3]

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3. Electronic Science & Technology Division, U.S. Naval Research Laboratory, USA

Nanocrystalline ceramics demonstrate property improvements over larger-grain-sized ceramics such as increased hardness, strength, and, potentially, damage tolerance. These property improvements result from "confinement" effects from the high degree of interfacial internal structure that influence modes of strain accommodation and crack propagation. Combining two or three different ceramic materials into a nanocrystalline composite ceramic provides the opportunity to further design the interfacial internal structure to create novel behaviors. Recent work at NRL has combined particle atomic layer deposition (pALD) with Environmentally Controlled – Pressure Assisted Sintering (EC-PAS) to synthesize dense nanocomposite ceramics from core-shell nanopowders. Limited experiments suggest that thermal properties of these nanocomposites do not follow simple rule-of-mixtures laws. Instead, thermal diffusivity is shown to be dominated by the constituent with a lower thermal diffusivity while thermal expansion falls outside that of either constituent, suggesting the need for a more comprehensive model to account for the macroscopic behavior.

Poster Session

Room: Orange C/D

5:30 PM

(EMA-P001-2022) Machine Learning Approaches to Predict Properties from Microstructure Images in Ceramic-Metal Composites

H. B. Smith*[1]; W. Huddleston[1]; L. Bruckman[1]; A. Sehirlioglu[2]

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

Electrical conductivity of composites of $Li_4Ti_5O_{12}$ anode and Ni current collector particles developed for structural battery applications were predicted from SEM microstructure images. Further, microstructural features contributing the most to conductivity for different samples could be identified. Principal component analysis (PCA) was performed on voronoi, nearest neighbor, size, and skeleton distributions of the microstructural features, and logistic regression and linear discriminant analysis models were fit to the scores of the principal components (PCs) to classify the images as low or high conductivity. Accuracies exceeded 87%, and the most important PCs were identified. Convolutional neural networks (CNN) were then used for classification and led to accuracies above 98%. Class activation maps were created from the CNN models for testing images. These highlight which microstructural features influenced conductivity predictions. Regression was attempted on the PCs using multiple linear regression and general additive models with little success. Regression attempts with CNN were unstable due to the sparsity of the data set but yielded responses that were usually 4x off the observed responses on average with values for r^2 usually exceeding 0.7.

(EMA-P002-2022) Fabrication and Characterization of an Additively Manufactured Thermoelectric Material

J. J. Potticary*[1]; B. Baker[1]; H. Elbidweihy[2]; E. Retzlaff[1]; P. Joyce[1]

1. United States Naval Academy, Mechanical Engineering, USA
2. United States Naval Academy, Electrical Engineering, USA

Additive Manufacturing (AM) is a method of manufacturing that involves the deposition of material vice the removal of a material to create a finished part. There are many different methods of AM. Of primary interest to this research is vat polymerization, specifically stereolithography (SLA). SLA uses a laser to cure a plastic resin. As the technology has developed researchers have created their own resins. These custom materials have even been doped with thermoelectric materials (TMats). The goal of this research is to use AM to fabricate a TMat and then characterize the thermoelectric and mechanical properties of that material. The research will investigate both the n and p variant of bismuth telluride. ZT, strength, fracture toughness, and hardness will be measured. The microstructure of the material as well as the composition of the material will also be analyzed. This research lays the foundation for the development of prototypes, and would provide valuable data for models in the future.

(EMA-P003-2022) Exploring Hindrances in Entropy Stabilization

K. E. Johnson*[1]; G. Niculescu[1]; E. Johnson[2]; L. J. Joyce[1]; K. Letchworth-Weaver[1]; C. M. Rost[1]

1. James Madison University, Physics and Astronomy, USA
2. James Madison University, Department of Geology and Environmental Science, USA

This study explores the phase evolution of bulk high entropy oxide composition $(MgCoNiCuSnZn)_{0.167}O$ at a lower temperature range using traditional solid-state synthesis methods. To gain a further understanding of what conditions will aid or impede single phase formation, $(MgCoNiCuSnZn)_{0.167}O$ was sintered from 700 °C to 1200 °C. The resulting samples were characterized by X-ray diffraction and SEM-EDS for phase and composition analysis, respectively. It appears that the introduction of the tin oxide into the system made formation of a single phase non-favorable. Understanding why entropy stabilization was hindered in this system, and others, will enable the possible solid-state synthesis of compositions other than the original $(MgNiCoCuZn)_{0.2}O$.

(EMA-P005-2022) Relaxor Behavior and Effect of Bi-Dopants in Barium Zirconate Titanate Solid Solutions as Energy Storage Materials

E. Kroell*[1]; D. C. Lupascu[1]; S. V. Vladimir[1]

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

The growing population and increasing global energy consumption in recent decades require advanced and miniaturized energy storage systems. Dielectric capacitors as energy storage systems are favorable due to their high power density and long life time, however they have low energy density. To increase the recoverable energy density, relaxor ferroelectrics are a promising group of materials because of their high dielectric permittivity and slim polarization hysteresis loops. To improve the energy storage performance of barium zirconate titanate $Ba(Zr_{0.15}Ti_{0.85})O_3$, we introduce bismuth compounds, $Bi(Zn_{2/3}Nb_{1/3})O_3$ and $Bi(Zn_{2/3}Ta_{1/3})O_3$. The heterovalent substitution at the A-site and B-site disrupts the long-rang order, while Bi^{3+} dopant improves the polarizability. The addition of Ta^{5+} should increase the breakdown strength of the ceramics to withstand higher electric fields and increase the recoverable energy density. The microstructure and phase characterization of the samples was investigated by scanning electron microscope and X-ray diffraction. For the dielectric properties and energy storage performance, impedance spectroscopy and polarization measurements were conducted.

(EMA-P006-2022) Emergent evolution of oxide superlattices and heterostructures: Thermal, optical, and electronic characterization via ultrafast spectroscopic methods

S. Hoseini Makrem*[1]; J. Tomko[1]; P. E. Hopkins[1]

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

Ravichandran et al demonstrated experimental evidence of the fundamental dynamics of phonon propagation in superlattices, a crossover from particle-like to wave-like. However, a detailed description of the related scattering processes for heterostructures with high interface density was unexplored. To complement this study, we perform a series of ultrafast laser spectroscopy measurements on the $(STO)_n/(CTO)_m$ superlattices. We perform Time-domain Brillouin scattering to interrogate the underlying changes in phonon dynamics. We find strong evidence for phonon localization corresponding to the thermal conductivity medium as individual layers begin to form a single emergent structure with octahedral tilts. Complementary to the evidence for evolution of structural regimes, we performed second harmonic generation (SHG). If there is an inversion symmetry in the constituent material, the higher rank dielectric tensor vanishes. Since both STO and CTO have inversion symmetry, the observed SHG intensity stems from the polarizability of the interface. Our results show that the structural transitions are directly reflected in the polarizability of the superlattices. As the heterostructure transitions from independent monolithic layers, to coupled layers, to a single centrosymmetric structure, the second-order optical response approaches zero.

(EMA-P007-2022) Acid-Base Reactions of Layered Perovskite Materials for Mechanical Exfoliation of Nanosheets

B. Hirt*[1]; A. Sehirlioglu[1]; M. Ornek[2]; C. Wernex[2]

1. Case Western Reserve University, Material Science and Engineering, USA
2. Purdue University, Mechanical Engineering, USA

Top-down approaches for creation of nanosheets allow scalability in processing and thus can enable a broader range of applications in comparison with bottom-up approaches. With proper processing,

large aspect ratios with thickness in the single digit nanometer ranges and lateral sizes in the micrometer range can be achieved. There has been a lack of in-depth systematic studies of obtaining protonated forms of the $Bi_{4+x}Fe_xTi_3O_{12+3x}$ family of Aurivillius phases. $Bi_4Ti_3O_{12}$, $Bi_5FeTi_3O_{15}$, and $Bi_6Fe_2Ti_3O_{18}$ were experimentally tested for the ability to synthesize protonated derivatives under a variety of experimental conditions. The protonated forms are created by reaction with strong acids causing an exchange of interlayer cations. The protonated structure can allow intercalation of bulky organic bases in the interlayers between perovskites, which weakens the forces between layers so that mechanical exfoliation can occur, creating nanosheets. In addition, protonated powders were shown as promising catalysts in a variety of applications such as combustion of ammonium perchlorate in solid state propellants and activation of peroxymonosulfate for bisphenol A degradation for water treatment.

(EMA-P008-2022) Preparation of new high-entropy perovskite-type oxides

G. Wang*[1]; D. C. Sinclair[1]; C. L. Freeman[1]; A. Nasrallah[1]

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

High entropy oxides (HEOs) have gained significant interest over the past few years due to their unique structural and functional properties. Multiple ions are occupied in one site to stabilise a single-phase crystal structure by increasing the configurational entropy of the system. However, some reported HEOs required special sintered techniques, i.e. spark plasma sintering, and may oftenly suffered from unstable crystal structure/phase after post-treatment procedures. Here, a new perovskite-type HEOs, $Ba(Ti_{0.2}, Sn_{0.2}, Zr_{0.2}, X_{0.2}, Nb_{0.2})$ with X^{3+} (Ga/Al/Sc/In), was synthesised successfully using solid-state reaction. By further reducing the number of B-site elements, as well as decreasing the configurational entropy of the system, single phases (cubic structure) of $Ba(X_{1/3}, Y_{1/3}, Nb_{1/3})O_3$ with X^{4+} (Ti/Sn/Zr) and Y^{3+}(Ga, In, Y, Sc) were also prepared successfully. Meanwhile, these HEOs retained the same phase after annealing procesure at 200 degreeC below sintering temperature.

(EMA-P009-2022) Electrical Characterization of Lithium Cobalt Oxide Nanosheets

B. Powers Beggs*[2]; K. Pachuta[2]; R. Vasudevan[1]; A. Sehirlioglu[2]

1. Oak Ridge National Lab, USA
2. Case Western Reserve University, USA

This presentation examines conductive atomic force microscopy measurements of cobalt oxide nanosheets taken between 325K and 500K. The data was converted into an HFD5 data format using the Pycroscopy package and analyzed in Python. Over 5,000 I-V curves were collected with -4.5 to 4.5V voltage sweeps along the nanosheets. Electrical conductivity information was extracted and processed for the samples and the substrate. The voltage curves were categorized as showing ohmic, insulating, rectifying, or back-to-back diode behavior and a mixture of these behaviors were observed during the scans as a function of x-y coordinate, expect at 500K where the behavior was almost exclusively ohmic, indicating that the materials became conductive at and above that temperature. The electrical behavior and conductivity was mapped to the 3D topography of the flakes.

(EMA-P010-2022) Rietveld Refinement of Neutron Diffraction Data of Li_xCoO_2

J. Frostad*[1]; K. Pachuta[1]; A. Sehirlioglu[1]

1. Case Western Reserve University, USA

$LiCoO_2$ (LCO) is treated with acid as the first step in the creation of cobalt oxide nanosheets. This step leads to both delithiation and protonation, neither of which is complete and their extent can affect the yield of processing as well as the final composition and defect structure of the flakes. Most studies on the acid treated LCO have used XRD which is not very sensitive to hydrogen content, limiting the characterization of protonation. In this study neutron diffraction data was obtained for LCO that underwent treatment with HCl at various concentrations ([HCl] = 0.1M, 0.3M, 1M, and 3M). The resulting structures were then analyzed using Rietveld refinement. The expansion in the c axis found from the refinement was in agreement with previous studies based on XRD. In addition, the Rietveld analysis was able to shed light on the protonation of the delithiated LCO structure. Texturing of the material was also taken into consideration as a potential variable in our analysis.

(EMA-P011-2022) Strain engineering and high resolution XRD of K_{1-x} Na_xNbO_3 thin films synthesized through aqueous solution deposition

M. Mahmoudvand*[1]; S. R. Burns[1]; A. Z. Mohammed[2]; M. Dolgos[1]

1. University of Calgary, Canada
2. University of calgary, Chemistry, Canada

One of the most promising lead-free piezoelectrics is potassium sodium niobate - K_{1-x} Na_xNbO_3 (KNN). Although functionality and properties of the material have been well studied in the bulk form of ceramics, little is known about how it behaves as a thin film. In this work, we utilize a process of isolating salts from commercially available chemicals (hydroxides and hydrated niobia) and forming highly ordered thin films on conducting ceramic substrates through simple heat treatment and spin coating. This deposition technique entirely avoids toxic precursors and/or hazardous waste by-products. New approaches to control the properties of potential devices will no doubt involve strain engineering, as the properties, especially piezoelectricity, of these films are greatly affected by the selection of host substrate. Therefore, one of our most promising approaches to control the properties of KNN is to deposit films on a range of different substrates for comparison of structure and electromechanical behaviour. Using high resolution x-ray diffraction (HRXRD) to collect reciprocal space maps (RSMs), we explore the structure of KNN films deposited on (001)- and (110)- oriented Nb:$SrTiO_3$, and (001)-oriented $LaAlO_3$. The results described are indicative of the flexibility afforded by this new aqueous deposition technique.

(EMA-P012-2022) Strain-induced 1D ferroelectricity in niobium oxide trihalides

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2. Pusan National University, Department of Physics, Republic of Korea

Switchable electric dipole at reduced dimension can be a breakthrough that overcomes the size limit of nanostructured electronic devices. Interestingly, Niobium chloride oxide ($NbCl_3O$) is a material that has been successfully fabricated in a one-dimensional Van der Waals(1D-vdW) crystal consisting of two parallel 1D nanowires. 1D nanowire in $NbCl_3O$ has a non-centrosymmetric structure but two parallel 1D nanowires are aligned anti-parallel to each other, which leads to an anti-ferroelectric bulk structure. Here, using density functional theory calculations, we report that a phase transition occurs from anti-ferroelectricity to ferroelectricity by biaxial strain. Our findings not only provide the possibility of 1D ferroelectrics but also suggest directions towards high-density ferroelectric devices.

(EMA-P013-2022) Synthesis and Characterization of a Novel Piezoelectric Material with a Morphotropic Phase Diagram

M. Dolgos*[1]

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We have recently synthesized a new "lead-lite" piezoelectric system with enhanced properties at the morphotropic phase boundary. This material is a solid solution between $PbTiO_3$ and a novel lead-free perovskite. The compositions in the MPB have a moderate Curie temperature and high d_{33}, similar to what is observed in $K_{0.5}Na_{0.5}TiO_3$. Here we will present the structural and physical properties as well as initial doping studies to tailor the properties for specific applications.

(EMA-P014-2022) Processing Structure Property Relationships in Hafnia-based Nanoparticles

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2. University of Florida, USA

HfO_2-based thin films are an emerging material for applications requiring nanoscale ferroelectricity. These thin films often can be composed of several crystal structures, primarily consisting of the ferroelectric orthorhombic phase with additional tetragonal and monoclinic phases. The stabilization of the ferroelectric phase has been attributed to composition (e.g., dopants/substitutional ions), surface energy, substrate induced film stress, and oxygen vacancies. Here, the phase space is explored for $Hf_xZr_{1-x}O_2$ (x=0.1-1) nanoparticles produced using a co-precipitation method to determine the effects of surface energy and composition on the formation of the orthorhombic, tetragonal, and monoclinic crystal structures. X-ray diffraction will be used to identify the effects of synthesis and processing parameters on the presence of different crystallographic phases in the synthesized nanoparticles. Methods on the fabrication and testing of $Hf_xZr_{1-x}O_2$-based nanoparticle composites for ferroelectric testing will also be presented.

(EMA-P015-2022) Growth of thin film lithium cobalt oxide for electrochemical studies

K. Gliebe*[1]; A. Sehirlioglu[2]

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

Lithium lanthanum titanate (LLTO) demonstrates high bulk ionic conductivity for use in solid state batteries; however, grain boundaries diminish LLTO's conductivity. We are aiming to understand the effects of ionic transport through the system when grain boundaries are not present and when the interface between the cathode and electrolyte is epitaxial. Targeted single crystal heterostructures are formed by layers of LLTO electrolyte / lithium cobalt oxide (LCO) cathode / strontium ruthenate (SRO), which acts as a buffer to form ohmic contact / substrate, strontium titanate (STO) and Nb:STO for two different configurations where the return interconnect will connect to SRO and the back of the substrate, respectively. Growth characteristics, structural evolution and the related properties were characterized as each layer was introduced (i.e., SRO conductivity as a function of thickness, LCO structure on SRO/STO etc.). In-situ reflection high energy electron diffraction, atomic force microscopy, and x-ray diffraction based techniques are coupled with electrical characterization to learn about the steps in building such hetero-structures.

(EMA-P016-2022) Sign reversal of tunneling magnetoresistance in all-oxide-based synthetic antiferromagnets

Z. Zhang*[1]

1. University of Science and Technology of China, Hefei National Laboratory for Physical Sciences at the Microscale, China

Magnetic multilayer devices that exploit magnetoresistance are the backbone of magnetic sensing and data storage technologies. Recently, all-oxide-based synthetic antiferromagnets (SAFMs) were synthesized by our group, which provides us an opportunity to study their tunneling magnetoresistance (TMR) and current-in-plane (CIP) MR. Here, using $CaRuO_3$ as the bottom electrode, Pt as the top electrode, and (001)-oriented $NdGaO_3$ as the substrate, we fabricated magnetic tunnel junctions based on manganite/ruthenate SAFMs, $[La_{2/3}Ca_{1/3}MnO_3(LCMO)(2.8\ nm)/CaRu_{1/2}Ti_{1/2}O_3(CRTO)(1.2\ nm)]_2$. Apart from the negative magnetoresistance of manganite thin films, the resistance of spin-dependent scattering depends on whether the same ultrathin ferromagnetic layers separated by an insulating layer are arranged anti-parallel or parallel. For the parallel case, the SAFMs show a relatively low TMR at low temperature, which is consistent with the two current model. As the temperature increases, a temperature-driven sign reversal of TMR occurs. However, when the ferromagnetic layers are antiferromagnetically coupled, the SAFMs have a lower CIP resistivity, which should be attributed to the carrier confinement effect caused by the half metallicity of the magnetic layers. This CIP MR, ~2‰, is one order of magnitude smaller than the corresponding TMR.

(EMA-P017-2022) Thermal Processing of Ceramic Thin Films via Pulsed Laser Annealing

N. A. Graham*[1]; R. J. Warzoha[1]; E. Patterson[2]; E. Gorzkowski[2]; B. F. Donovan[1]

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2. Naval Research Lab, USA

Thermal processing of typical thin film ceramic samples is generally done in a large scale environment such as an oven or furnace, which heats an entire sample uniformly. In order to achieve novel thermal processing configurations, we move to thermal processing using pulsed laser annealing (PLA). In this project, we intergoate the effects of heat deposited by an excimer laser on thin films of functional oxides. Results include influence of pulsed laser heating on grain growth in fine grained films and may be extended to utilizing PLA in the pyrolisi and annealing steps of chemical solution deposition. Thermal treatment paramters are guided by COMSOL models.

(EMA-P018-2022) Toward Video Rate Visualization of Ferroelectric Domains by Friction Asymmetry

S. Cho*[1]; I. Gaponenko[2]; K. C. Edwards[2]; E. Cho[1]; L. Musy[2]; J. Yeom[1]; C. Lichtensteiger[2]; P. Paruch[2]; S. Hong[1]

1. Korea Advanced Institute of Science and Engineering (KAIST), Materials Science and Engineering, Republic of Korea
2. University of Geneva, DQMP, Switzerland

High-speed characterization and control of localized grains, domains, and their boundaries have great importance for understanding structure-property relationship and engineering the properties of ferroelectrics. Piezoresponse Force Microscopy (PFM) is one of the well-established SPM techniques that can visualize and control ferroelectric domains using converse piezoelectric effect, i.e based on electromechanical 'coupling'. In this technique, converse piezoelectric strain through the conductive nanoscale probe allows ferroelectric domain to be visualized after extracting amplitude and phase signals by lock-in amplifier. However, the speed of visualization is limited by resonance frequency of cantilever and the time constant of lock-in amplifier. Furthermore, the electrostatic effect through localized probe can induce artifacts in the PFM images. Here, low-cost, faster, and voltage-free visualization of polarization domains using scanning probe microscopy has been demonstrated in ferroelectric thin film without any signal amplifier. A strain gradient induced polarization component leads to asymmetric signal in lateral force microscopy (LFM) and local friction imaging thus gives direct information on up and down polarization domains at high scan rates beyond 4 FPS. We envision that this high-speed imaging can be useful for the investigation of polarization dynamics and big data acquisition.

(EMA-P019-2022) Structural design for high performances and high durability of copper oxide photoelectrodes

D. Kim[1]; H. Cho*[1]

1. Sungkyunkwan University, Republic of Korea

Among several sustainable alternatives, solar energy may be the most efficient solution because it constitutes the largest renewable energy source. In various solar energy to power conversion systems, the photoelectrochemical (PEC) splitting of water into hydrogen and oxygen by the direct use of solar energy is an ideal process. It is a renewable method of hydrogen production integrated with solar

energy absorption and water electrolysis using a single photoelectrode. Our photoelectrodes are based on low-cost copper elements and p-type oxide. The copper oxides have been studied as a good candidate material for PEC operation for a long time. Nevertheless, they showed insufficient photocurrents and not robust chemical durability. The use of protective layers for chemical durability reduces the photocurrent values essentially. Thus, photocurrent and long-term operation should be compromised. In our study, we suggest a new concept focusing on structural design for the simultaneous guarantee for photocurrent and stability, which includes additional layers and surface treatment.

(EMA-P020-2022) First-principle Study of Interplay Between Flat and Dirac Band

M. Kang*[1]; Y. Jin[1]; J. Lee[1]

1. Pusan National University, Department of Physics, Republic of Korea

Pyrochlore oxides denoted by $A_2B_2O_7$ (or $A_2B_2O_6O'$) have been attracting much attention due to the coexistence of flat and Dirac bands around the Fermi energy. It has been known that the flat bands are originated from the orbital interactions of the geometrically frustrated pyrochlore lattice similar to 2D checkerboard and Kagome lattice, while the Dirac bands are related to the Sn-s orbital. Here, using the first-principles density functional theory calculation, we investigate the interplay between Flat and Dirac bands in $Sn_2Nb_2O_7$ oxide by applying biaxial strain and considering substitutional doping in A-site sublattice. Emergence of long-range magnetic order and novel magnetic ground state will be discussed in detail along with atomistic study of strong interaction between Flat and Dirac band in $Sn_2Nb_2O_7$ oxide.

(EMA-P021-2022) Conductivity trends & mechanisms in heavily acceptor doped Pb(Zr,Ti)O_3

V. Sangwan*[1]; M. Bowen[2]; D. Cann[2]

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The ferroelectric and piezoelectric properties of lead zirconate titanate (PZT) have led to numerous applications, such as sensors, actuators, and high-value ceramic capacitors. This study is focused on the AC and DC conductivity of PZT ceramics with a Zr/Ti ratio of 50/50 that incorporates high levels of acceptor doping (i.e., greater than 10 mol% Fe). Ceramics were synthesized using solid-state processing techniques with an observed acceptor dopant solubility limit of 6 mol% Fe. X-ray diffraction and dielectric measurements revealed a tetragonal structure at room temperature with a phase transition at 390°C. Increased levels of Fe-doping resulted in a decrease in the Curie temperature with T_c = 350°C for 5% Fe. Conductivity measurements using AC electrochemical impedance spectroscopy showed an increase in bulk conductivity with increased Fe-doping up to 20 mol% Fe. AC electrical conductivity measurements were validated using DC resistance measurements with a bulk Van der Pauw geometry. For 5% Fe-doped PZT around 450C, the conductivity was found to be 5.9 S/cm with AC methods versus 5.5 S/cm with DC measurements. While acceptor doped PZT has been studied extensively for the hardening effect in piezoelectric applications, this work examines the effects of high levels of acceptor doping on the conductivity of PZT which may be useful for oxygen-ion conducting applications.

(EMA-P022-2022) Exploring point defects and trap states in undoped $SrTiO_3$ single crystals

M. Siebenhofer*[1]; F. Baiutti[2]; M. Liedke[3]; J. Fleig[1]; M. Kubicek[1]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria
2. IREC, Nanoionics and Fuel Cells, Spain
3. Helmholtz-Zentrum Dresden-Rossendorf, Nuclear Physics, Germany

$SrTiO_3$ (STO) is a mixed conducting perovskite oxide, and its properties are exploited in a multitude of devices. Well established defect models exist for acceptor- and donor-doped STO, however, establishing a model for undoped single crystals is challenging due to the potential presence of various equally concentrated intrinsic defects and impurities down to ppm levels. In this contribution, we present a method capable of sub-ppm defect analysis, based on investigations of the chemical capacitance. By detailed measurements of the low frequency impedance response of nominally undoped STO single crystals, measured in a wide $p(O_2)$ range at intermediate (500-700 °C) and low temperatures (25-180 °C), it was possible to establish a defect model for undoped STO purely based on electrochemical measurements. In addition to defect concentrations, our method also allows to determine electronic trapping energies, e.g. of electron holes trapped at cation vacancies. From detailed analysis of the measured impedance response and positron annihilation lifetime spectroscopy (PALS), it was possible to consistently determine an acceptor dopant concentration of 6 ppm Ti vacancies. Trace elemental analysis (by ICP-MS) further indicated the presence of Al impurities (sub-ppm) and allowed to measure the concentration of uncharged impurities such as Ba and Ca on the Sr-site which are not accessible by our electrochemical method.

(EMA-P023-2022) Surface decoration of $Pr_{0.1}Ce_{0.9}O_{2-\delta}$ electrodes with binary oxides measured by in-situ PLD technique

C. Riedl*[1]; M. Siebenhofer[1]; A. Limbeck[1]; A. K. Opitz[1]; M. Kubicek[1]; J. Fleig[1]

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria

Improving mechanistic understanding of the oxygen reduction reaction (ORR) taking place on the surface of SOFC cathodes is a major goal of current research. In this contribution, $Pr_{0.1}Ce_{0.9}O_{2-\delta}$ (PCO) electrodes were grown as dense thin films by pulsed laser deposition (PLD) and were characterized directly after growth via impedance spectroscopy inside the PLD chamber (i-PLD), which enables quantification of the oxygen reduction kinetics on contaminant-free surfaces unaltered by any external degradation. The unusually high stability of the polarization resistance allows us to study electrode kinetics at different $p(O_2)$ and temperatures, thus leading to interesting mechanistic insights. In this study, the electrode surface of PCO was decorated with sub-monolayer amounts of different binary oxides. i-PLD measurements offered us the advantage to directly track changes of the impedance upon decoration with every single deposited pulse of the respective binary oxide. In accordance with the results of Nicollet et al., our measurements show that acidic oxides (SnO_2, TiO_2) led to a significant increase of the polarization resistance, while basic oxides (SrO, CaO) accelerated the ORR kinetics. Most interestingly, no change of the $p(O_2)$ dependence and activation energy was observed, which indicates that despite changes in surface chemistry, the rate limiting step remains unchanged.

(EMA-P024-2022) First-principles investigation on the physical origin of the electro-plasticity of metals

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It is known that the plasticity of metals enhances under electric current. This electro-plasticity has been utilizing in the materials industry for various purposes. It has been regarded to originate from the Joule's heating by the current. Intriguingly, it was, however, found that the temperature rising caused by the current is not sufficiently high to explain the phenomenon. We perform the

first-principles calculations to explain the physical origin of this electro-plasticity. We focus our investigation on the effects of extra charges supplied by the current on phonon properties and shear deformation. Our calculations reveal that a small amount of charge does not change the phonon properties of the perfect bulk structures. In imperfect structures, such as slabs with surfaces and structures with grain boundaries, on the other hand, some of their phonon modes become softened by charging. In addition, we find that shearing energy barriers of various metal slabs reduce in certain charging conditions. We attribute the electro-plasticity to charge accumulation either positively or negatively, which eventually provokes stress in metals resulting in the enhancement of plasticity.

(EMA-P025-2022) A novel method to calculate size-dependent conductivity of metal interconnects based on modified relaxation time

J. Lee*[1]; Y. Lee[1]; S. Lee[1]; Y. Kwon[1]

1. Kyung Hee University, Department of physics, Republic of Korea

The modern CMOS technology begins to encounter several critical issues, including quantum size effects as well as interconnects, the resistivity of which increases with downscaling. Until now, Copper has been regarded as the best material for the interconnect thanks to its low resistivity, but its resistivity drastically increases when circuits have been miniaturized. There have been lots of efforts to find new interconnect materials, the resistivity of which becomes eventually smaller than that of copper after experiencing a crossover point in the plot of the resistivity as a function of device size. Various materials have been proposed to replace copper interconnect based on the FS theory, which somewhat empirically considers the size effects by evaluating bulk resistivity and electron mean free path, but without considering quantum mechanical effects of electronic transport properties. We develop a method to evaluate the carrier relaxation time as a function of the band index and electron momentum modified by surface boundary scattering, which is then provided into the Boltzmann transport equation to solve the size-dependent resistivity. We apply our method to various metals including single, binary elemental metals and MAX phase materials, to search for novel interconnect materials replacing copper in future electronics.

(EMA-P026-2022) Ab initio Study on the Structural and Electronic Properties of Interfacial Phase-Change Memory

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2. Yonsei University, Department of Physics and Applied Physics, Republic of Korea

Recently, interfacial phase-change memory composed of Ge, Sb, and Te (GST) has been introduced as a promising candidate for the next-generation nonvolatile memory, because of its low power consumption and fast response time. Although these features are evident and reproducible, the phase change mechanism including even its metastable structure has not been revealed yet. To tackle this unknown problem, we investigate its structural and electronic properties using ab initio calculations based on the density functional theory. Guided by the TEM images, we find that the low resistance state mainly originates from the hexagonal Ge_3Te_4-Sb_2Te_3 superlattice, whereas the high resistance state does from intermixed cubic structures of GST. Such structural distinction is confirmed by calculated XRD spectra and used to explain the peak shift observed in XPS. It is also found that the mobility of Ge atoms is much higher than that of Sb atoms by evaluating their diffusion barriers fed to the Arrhenius equation. Therefore, the phase change process between the low and high resistance states is mainly attributed to the Ge diffusion. We propose a possible diffusion scenario describing the phase change process. We also solve the Boltzmann transport equation to estimate the electric conductivity of the high resistance state to be one or two orders of magnitude lower than that of the low resistance state.

(EMA-P027-2022) Magnetic anisotropy energy of Fe layers controlled by various perovskite ABO3 substrates

D. Jeong*[1]; Y. Kwon[1]

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Although CMOS-based conventional semiconductor devices have recently been miniaturized up to a 5 nm process, there are still various quantum mechanical limitations to be tackled. Typical examples are a quantum tunneling effect and high switching energy demanded. To overcome these limitations, spin-based devices have been rapidly developed over the past few decades. A novel spintronic device was proposed based on two main mechanisms: spin-charge conversion and spin switching of a ferromagnetic made of La-doped $BiFeO_3$, a multiferroic material. Later, instead of this multiferroic material, which is difficult to manufacture as a thin film, a soft magnetic cladding structure was proposed for ferromagnetic switching. The key issue is how to lower magnetic anisotropy energy and thus making switching easier. Using the first-principles density functional theory, we investigate the magnetic properties of Fe layers stacked on various ferroelectric oxides ABO_3, where A is one of the alkaline earth metals (Ca, Sr, or Ba) and B is a transition metal in the titanium group (Ti, Zr, or Hf). We explore the effects of the spontaneous polarization of ABO_3 as well as of different elements A and B on the magnetic anisotropy energy of the Fe layers and suggest which system will be most efficient for lowering the magnetic anisotropy energy.

(EMA-P028-2022) Resistive switching in Au/Nb:STO junctions under different environments

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1. Los Alamos National Lab, USA

Metal oxide-based resistive switching (RS) devices have demonstrated huge potentials for non-volatile memory and computing technologies. However, the role of various ambient environment on the RS of metal/metal-oxides interface has not been studied yet. We used Au/Nb:STO as a model system to study the role of switching environment and interface quality on RS properties. For the switching environment effect, we investigated RS in various conditions such as ambient and gas (N_2 and O_2) environment. It was found that the RS in Au/Nb:STO depends strongly on the environment. For the interface quality effect, we treated Nb:STO in different temperatures, the RS behavior also strongly depends on the annealing conditions. The work has concluded the critical roles of oxygen vacancy and trapping/detrapping in RS for the Au/Nb:STO system.

(EMA-P029-2022) Reversible polarization switching in leaky ferroelectrics using an ionic gel induced electrostatic field effect

S. Huang*[1]; F. Blom[1]; G. Koster[1]; G. Rijnders[1]

1. University of Twente, TNW, Netherlands

In this work, a transparent and free-standing ionic gel as the dielectric layer for polarization switching in leaky ferroelectric thin films is reported. Applying an electric field over an ionic liquid dielectric layer used as an electrostatic field gated capacitor one can avoid electronic conduction. The association of electrical double layer (EDL) with depolarization at the solid-liquid interface contributes to the successful reversible switching in PbZrxTi1-xO3 (PZT). Using such ionic gels, the anisotropic ferroelastic switching from monoc-domain towards a-domain is studied in PZT grown on CaF2 substrates. Our results demonstrate that an electrostatic field, induced by the free-standing ionic gel is an effective and promising way to investigate leaky ferroelectrics.

Thursday, January 20, 2022

Plenary Sessions

Plenary Session II

Room: Orange A
Session Chair: Wolfgang Rheinheimer, Jülich Research Ceter

8:40 AM

(EMA-PLEN- 002-2022) Energy-Efficient Hardware and Intelligent Materials for Brain-inspired Computing: Artificial Synapses Based on Proton and Oxygen Motion

B. Yildiz*[1]

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Deep learning is a powerful algorithm for machine learning applications such as computer vision and natural language processing. However, the training of these neural networks is limited by the traditional von Neumann architecture of our current CPUs and GPUs. Shuttling data back and forth between the separate memory and computation units in such architecture results in significant energy consumption; many orders of magnitude greater than the energy consumption in human brain. In our research, we aim to reduce the energy consumption in analog, brain-inspired computing, by focusing on designing materials and devices that can instead perform data storage and computation in a single architecture using ions. First, I will share our work on a protonic electrochemical synapse concept that changes conductivity deterministically by current-controlled shuffling of dopant protons across the active device layer; resulting in energy consumption on par with biological synapses in the brain. Second, I will share our work in controlling the consistency of conducting oxygen vacancy filament formation in resistive memory devices via dopant and microstructure engineering. These strategies provide pathways towards brain-inspired hardware that has high yield and consistency and uses significantly lesser energy as compared to current computing architectures.

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

Advanced Electronic Materials, including Ferroelectric, Piezoelectric, Dielectric, Electrostrictive, and Pyroelectric Materials III

Room: Citrus A

10:00 AM

(EMA-097-2022) Solid-state crystal growth of (K,Na)NbO_3 and (K,Na)NbO_3-based single crystals (Invited)

I. Fujii*[1]; S. Ueno[1]; S. Wada[1]

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Lead-free piezoelectric materials have been studied for the environmental concern. (K,Na)NbO_3 is one of the intensively studied lead-free materials, because piezoelectric properties comparable to those of Pb(Zr,Ti)O_3 can be obtained by elaborate compositional modifications. To further increase its piezoelectric properties, the fabrication of single crystals is effective. However, the growth of $(K_{0.5}Na_{0.5})NbO_3$ and $(K_{0.5}Na_{0.5})NbO_3$-based single crystals with homogenous chemical compositions by conventional melt growth and solution growth methods is difficult because of the incongruent melting of $(K_{0.5}Na_{0.5})NbO_3$. In this study, the single crystals of $(K_{0.5}Na_{0.5})NbO_3$, (Li,K,Na)NbO_3, and (Li,K,Na)NbO_3-$BaZrO_3$-$(Bi_{0.5}Na_{0.5})TiO_3$ with homogenous chemical compositions were fabricated by a solid-state crystal growth method with a $KTaO_3$ seed crystal. First, the effects of sintering aid material and content, atmospheric powders, sintering temperature and time, and the orientation of the seed crystal on the crystal growth of $(K_{0.5}Na_{0.5})NbO_3$ single crystals were investigated. Then, electric properties were measured for selected single crystal samples. It was found that the properties were comparable with those of reported (K,Na)NbO_3 single crystals fabricated by other growth techniques. The results of (Li,K,Na)NbO_3 and (Li,K,Na)NbO_3-$BaZrO_3$-$(Bi_{0.5}Na_{0.5})TiO_3$ single crystals will also be presented.

10:30 AM

(EMA-098-2022) Electromechanical Coupling in AlN and $Sc_xAl_{1-x}N$ Films Grown by Plasma-Assisted Epitaxy on Various Metallic Seed Layers and Substrates

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Piezoelectric aluminum nitride (AlN) or scandium aluminum nitride ($Sc_xAl_{1-x}N$) thin films offer potential flexibility for use in multiple substrates over bulk piezoelectric single crystal typically used in wireless Surface Acoustic Wave (SAW) sensors and other electromechanical devices. These materials remain piezoelectric at least to 800°C and can be synthesized in thin film form by magnetron sputtering or plasma-assisted epitaxy. Reports by several groups indicate that the magnitude of piezoelectric response can be optimized by growing (0002) textured AlN or $Sc_xAl_{1-x}N$ films on single crystal sapphire, Si, GaN, or SiC substrates. Growth of piezoelectric AlN and $Sc_xAl_{1-x}N$ films directly onto metallic substrates will enable improved flexibility in utilizing SAW sensors and other AlN-based devices for industrial monitoring. In this work, piezoelectric AlN and $Sc_xAl_{1-x}N$ films were grown by plasma-assisted epitaxy on seed layers including Pt, Zr, and Ti on c-sapphire as well as on bulk metal surfaces including Mo, steel and Inconel with and without the use of an AlO_xN_y buffer layer. SAW resonators (SAWRs) and SAW delay-lines operating near 450MHz were fabricated and used to measure the film electromechanical coupling coefficients, k^2. The results indicate a correlation between the metallic seed-layer choice and the degree of piezoelectric response.

10:45 AM

(EMA-099-2022) Dielectric permittivity study of $AgNbO_3$ antiferroelectric multilayers for use at high electric fields and temperatures

L. Fulanovic*[2]; M. Zhang[2]; N. Novak[3]; J. Koruza[1]; J. Rödel[2]

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2. Technische Universität Darmstadt, Germany
3. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia

Interest in the application of antiferroelectric (AFE) materials is rising, an example referring to the utilization of AFEs in commercially available DC-link or high voltage capacitors. These devices exploit the distinctive behavior of AFEs: an increased dielectric permittivity (ε) with increasing DC bias field. However, systematic study of ε with DC bias at high temperatures is still missing for any of AFEs. In this work, we present multilayer ceramic capacitors (MLCC) prepared using $AgNbO_3$ powder. Tape casting was used to fabricate MLCC structure, which consists of nine 40 µm thick ceramic layers. Double polarization vs. electric field loops were obtained at 17 kV/mm and 25 °C, and were stable up to 175 °C. Moreover, in the same temperature range the energy storage density increased from 1.5 to 2.5 J/cm^3. Permittivity ε exhibited an increase upon the application of DC bias field, which maximizes at the AFE to FE phase transition. The ratio between the permittivity value at 0 kV/mm and that at the phase transition point was found to increase even more significantly with temperature, in the range of up to 225 °C. This work provided sufficient data for the construction of the

electric field versus temperature phase diagram of $AgNbO_3$, which offers a detailed insight into the complex ε behavior as a function of electric field and temperature.

11:00 AM

(EMA-100-2022) Lead-free and antiferroelectric ceramics for novel energy and heat-management technologies

Z. Kutnjak*[1]; B. Rozic[2]; Z. Hanani[6]; S. Merselmiz[6]; D. Mezzane[6]; M. El Marssi[3]; H. Uršič[4]; M. Spreitzer[5]

1. Jozef Stefan Institute, Slovenia
2. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia
3. Université de Picardie Jules Verne, LPMC, France
4. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia
5. Jozef Stefan Institute, Advanced Materials, Slovenia
6. Cadi Ayyad University, IMED-lab, Morocco

The request for greener heat-management technologies has recently developed a significant interest in new electrocaloric (EC) effect-based cooling devices that can replace the existing cooling technics. An overview of experimental and theoretical investigations of the large EC and piezoelectric response in lead-free ceramic composites and ceramics near antiferroelectric transition will be presented in this contribution. Specifically, the large EC response observed by direct experiments in lead-free BCTZ-based ceramics will be reviewed, including the large energy harvesting potential in polymer composites. Besides, it is demonstrated that both negative and positive EC responses can be arbitrarily invoked in antiferroelectric materials by properly controlling the electric field and temperature, which enables enhancement of the electrocaloric cooling power for up to 100%.

11:15 AM

(EMA-101-2022) Direct observation on the ferroelectric-antiferroelectric transition in $Pb(Nb,Zr,Sn,Ti)O_3$/ZnO ceramic composites

B. Liu*[1]

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

$(1-x)Pb_{0.99}\{Nb_{0.02}[(Zr_{0.57}Sn_{0.43})_{0.937}Ti_{0.063}]_{0.98}\}O_3$ (PNZST)/xZnO ceramic composites were recently reported to display an ultrahigh pyroelectricity near human body temperature due to the ferroelectric - antiferroelectric transition of the matrix grains. In the present work, an in-situ TEM heating study is conducted on two composites of x = 0.1 and 0.4. The presence of strain field in the PNZST grain adjacent to a ZnO particle is verified. The stabilized ferroelectric phase at room temperature in the composite of x = 0.1 is noticed. The ferroelectric matrix grain transforms to the antiferroelectric phase in heating process and leads to the pyroelectric effect. In the composite of x = 0.4, advanced TEM analysis reveals the existence of both ZnO and Zn_2SnO_4. The formation of Zn_2SnO_4 indicates that parts of the Sn in the PNZST matrix grain is extracted and decomposition of the perovskite phase has taken place. Fine particles generated by the matrix grain decomposition products are observed, which assists the nucleation of the antiferroelectric phase and impedes the movement of the phase boundary. The much lower pyroelectric coefficient in the x = 0.4 composite is likely to come from the larger amount of ZnO and Zn_2SnO_4 and the decomposition of the PNZST perovskite phase.

11:30 AM

(EMA-102-2022) Stability of piezoceramic materials at high power drive (Invited)

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Piezoceramics are widely used in ultrasonic motors, cutting/welding, cleaning baths, medical ultrasound, and voltage transformers. Here, the piezoceramic elements are driven near their resonant frequency by a high AC electric field that produces a high vibration velocity. These conditions require piezoelectrically hard materials with low losses and high coupling factors. Extrapolation of small-signal parameters to high-power conditions does not reproduce the experimental observations and is thus inappropriate. We have investigated the high-power behavior of various hard piezoceramics, including $Pb(Zr,Ti)O_3$, $Na_{1/2}Bi_{1/2}TiO_3$-$BaTiO_3$, and $BaTiO_3$, which were hardened by either acceptor-doping or composite approach. Large-signal parameters were determined by the Burst excitation method, while the intrinsic/extrinsic contributions to the strain were measured in situ using high-energy X-ray diffraction. We show that the main driving force for domain wall motion is the dynamic mechanical stress. The small-signal parameters are not maintained under large-signal conditions; the former being stronger influenced by the hardening mechanism. The high-power stability could be related to the inherent material's behavior and the extent of the lattice contribution to strain. This intrinsic contribution was found to be 80-95 % for $Pb(Zr,Ti)O_3$ and 95-97 % for $Na_{1/2}Bi_{1/2}TiO_3$-$BaTiO_3$, explaining the excellent high-power stability of the latter.

12:00 PM

(EMA-103-2022) Aerosol Deposition and Characterization of Sodium Niobate

E. Patterson*[1]; J. Wollmershauser[2]; E. Gorzkowski[1]

1. Naval Research Laboratory, USA
2. U.S. Naval Research Laboratory, Materials Science & Technology Division, USA

Aerosol deposition was used to produce thick-films with layer thicknesses between 10 to 50 microns. The bonding and densification of the film and film/substrate interface facilitated by high pressure, impact and fracture of the particles. The films have microstructures characterized by XRD to have nano-grained crystallites and have been shown to have high residual stresses. This inhibits the formation of ferroelectric domains even in the prototypical ferroelectric system of barium titanate, which correlates to the well-known grain size effect in bulk ceramics. Due to these high residual stresses, materials systems that exhibit either antiferroelectric properties in the bulk (such as $NaNbO_3$) are natural alternatives to be studied via this technique. Deposition was performed onto thin metal foil substrates to facilitate the characterization of the electrical properties of the films.

12:15 PM

(EMA-104-2022) pO2-Mediated Transport as a Means for Structural and Electronic Tunability in Entropy Stabilized Oxides

V. Jacobson*[1]; D. Diercks[1]; B. To[2]; K. Gann[1]; A. Zakutayev[2]; G. L. Brennecka[3]

1. Colorado School of Mines, USA
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3. Colorado School of Mines, USA

Entropy stabilization in ceramics has gained significant attention in recent years as a means to engineering novel materials. In a multi-variable investigation of polycrystalline $(Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})O$ thin films deposited via pulsed laser deposition (PLD), it is shown that substrate temperature and deposition pressure have strong and repeatable effects on film texture and lattice parameter. Current density measurements and further analysis show that samples grown under reducing conditions are ~40x more electrically conductive than otherwise identical films grown at higher temperature and pressure. This electronic conductivity is hypothesized to be the result of polaron hopping mediated by transition metal valence changes which compensate for oxygen off-stoichiometry. Further study in bulk samples and their processing conditions reveals that the kinetics of sintering are also greatly affected by oxygen content. Using this knowledge, it is possible to sinter >97% dense bulk samples with a high pO2 atmosphere and kinetically optimized heating profile.

Materials Design, New Materials and Structures, and their Emerging Applications / Reliability and Fatigue of Ferroelectrics and Related Devices

Room: Citrus A

2:00 PM

(EMA-141-2022) Thermodynamic Phase Equilibria in the Nb_2O_5 — TiO_2 Binary System and Associated Ferroelectric Applications

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The high-temperature monoclinic phase of Nb_2O_5 has potential for applications that require high dielectric permittivity. Like its chemical relative Ta_2O_5, Nb_2O_5 has indications of large dielectric constants when alloyed with several mol% of aliovalent cations like Al, Si, and Ti. While incompletely known, lattice distortions or symmetry changes due to low mol% additions of metal cations may induce additional mechanisms of polarity within the single-phase solid solution monoclinic Nb_2O_5. For the system TiO_2 - Nb_2O_5, the bulk phase diagram suggests a solid solution region between 0% and ~8% Ti. However, this phase boundary is only projected in the literature and has yet to be experimentally verified. In addition, there are multiple reports of low mol% Ti intermediate compounds, e.g., $TiNb_{12}O_{29}$, which are incompletely documented. In the present work, we map this compositional space at high temperatures using X-ray diffraction to identify the two-phase to single-phase transition in quenched ceramics and thin films. Additionally, we report lattice parameter observations and corresponding electronic properties in low-TiO_2 concentration systems to assess the viability of this system in the context of ferroelectric applications. Current experiments reveal a solubility limit in the vicinity 5 mol% TiO_2 and crystal structures consistent with either monoclinic Nb_xO_y or $NbTi_{12}O_{29}$.

2:15 PM

(EMA-143-2022) Synthesis of α-MoO_3 Crystals via Chemical Vapor Transport for Directional and Hypersonic Heat Flow

R. Spangler*[1]; J. Caldwell[2]; A. Cleri[1]; K. Diaz-Granados[2]; P. E. Hopkins[3]; J. Tomko[3]; D. Hirt[3]; J. Maria[1]

1. Pennsylvania State University, Materials Science and Engineering, USA
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Orthorhombic molybdenum(VI) oxide, α-MoO_3, is a large-band gap semiconductor that exhibits numerous optical and electronic qualities conducive for applications in electronics, field-emission devices, light-emitting diodes, and various other devices. In the field of plasmonics, α-MoO_3 is of particular interest due to the three-dimensional optical anisotropy of the layered structure, in contrast to most alternative materials such as hexagonal BN which exhibit anisotropy along only two axes. Therefore, in certain spectral bands, the propagation of hyperbolic polaritons, or the coupled transport of light, heat, and charge oscillations, can restrict energy flow along a single crystal direction. This "energy beaming" phenomenon may enable hypersonic thermal transport towards precisely engineered locations in electronic and optical systems, dramatically altering thermal management in these devices. Here, α-MoO_3 crystals are synthesized using a chemical vapor transport technique, which has been identified as an effective approach for growth of these layers. We present structural, optical, and microscopic data characterizing the formation of α-MoO_3 crystals under various growth parameters.

2:30 PM

(EMA-144-2022) Modulation of the Bi^{3+} $6s^2$ lone pair state in perovskites for high-mobility p-type oxide semiconductors

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2. Xiamen University, College of Chemistry and Chemical Engineering, China

Oxide semiconductors are key materials in many fields from flat-panel displays to transparent electronics. However, many potential applications are still hindered by the lack of high mobility p-type oxide semiconductors due to the localized nature of O 2p derived valence band (VB) structure. Here we report on the modulation of the VB structure of perovskite Ba_2BiMO_6 (M= Bi, Nb, Ta) via the Bi $6s^2$ lone pair state to achieve p-type oxide semiconductors with high hole mobility up to 20 $cm^2 V^{-1} s^{-1}$, and optical bandgaps widely varying from 1.5 to 3.2 eV. We used PLD to grow high quality epitaxial thin films. Combined hard x-ray PES, XAS and DFT calculations were used to gain insight into the electronic structure responsible for the appealing properties of Ba_2BiMO_6. The high mobility is attributed to the highly dispersive VB edges contributed from the strong coupling of Bi 6s with O 2p at the top of VB that lead to low hole effective masses. Variation in bandgaps results from the change in the energy positions of unoccupied 6s orbital of Bi or d orbitals of Nb/Ta that form the bottom of CB. Ba_2BiMO_6 has compatible structures with many n-type counterparts, giving the possibility to fabricate high-quality devices. Our work provides deep insight into the electronic structure of Bi^{3+} based perovskites and guides the development of new p-type oxide semiconductors for optoelectronics.

2:45 PM

(EMA-145-2022) Research on Electro-Thermodynamic Cycle Power Generation with multifaceted analysis

H. Tanaka*[1]; T. Nagatani[1]; S. Yamaguchi[1]; T. Ichikawa[1]; H. Hashimoto[2]; T. Sekino[3]; T. Kawasaki[5]; M. Baba[4]; M. Takeda[4]; T. Nakayama[4]

1. Kwansei Gakuin University, Nanotechnology for Sustainable Energy, Japan
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4. Nagaoka University of Technology, Japan
5. Japan Atomic Energy Agency, Sector of Nuclear Science Research, Japan

Significant reduction of CO_2 has become an urgent issue to stop global warming, and various efforts have been made to make effective use of energy. Above all, the waste heat energy of the industry from power plants and factories is as large as the amount of electric energy produced by domestic power plants. Therefore, it is desirable to regenerate waste heat, especially from low-grade waste heat below 200 °C, which was difficult to regenerate with conventional technology. We have been researching a new "Electro-Thermodynamic Cycle Power Generation" that converts temporal temperature changes into electrical energy using ferroelectric materials. Aiming for a wider range of applications, we are working on the development of lead-free materials, and the development focusing on $BaTiO_3$ type ceramics is underway. In this $BaTiO_3$ type ferroelectric substance, very interesting results were obtained that the power generation performances were significantly different between pure $BaTiO_3$ and doped-$BaZrTiO_3$. Here, not only crystal analysis such as X-ray Diffraction (XRD) and Neutron diffraction (ND), but also multiple analysis methods such as Differential Scanning Calorimeter (DSC), Electro-Caloric Effect (ECE), and Atomic Force and Piezo-Response Microscopies (AFM-PRM) were used to study the power generation mechanism from various aspects. [Acknowledgement] A part of this work was supported by NEDO, Japan

3:00 PM

(EMA-146-2022) Photocatalytic activity of magnetically separatable N-doped rGO/$NiFe_2O_4$@Ti-doped ZnO ternary nanocomposite

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The N-doped rGO/$NiFe_2O_4$@Ti-doped ZnO as a novel ternary nanocomposite with magnetic recyclable was obtained by hydrothermal method. The structure, morphology, and optical as well as magnetic properties of synthesized nanocomposite were analyzed using the XRD, FTIR, Raman spectroscopy, FESEM with EDS, TEM, UV-vis DRS, and VSM. The photocatalytic activity was determined by the degradation of Methylene blue and Methylene orange dyes under visible light irradiation. The XRD and FTIR analyses confirmed that ternary nanocomposite was thoroughly synthesized. FESEM and TEM images indicated that $NiFe_2O_4$@Ti-doped ZnO nanospheres were embedded on N-doped rGO nanosheets. The band gap energies of pure ZnO, $NiFe_2O_4$@Ti-doped ZnO, and N-doped rGO/$NiFe_2O_4$@Ti-doped ZnO were calculated 3.19 eV, 2.44 eV, 1.88 eV via UV-vis spectra, respectively. Thus, the band gap of ternary nanocomposite became narrowing and exhibited better optical property. The result of the photocatalytic test showed 98% and 99% MB and MO degradation under 440 min visible light, respectively, in presence of N-doped rGO/$NiFe_2O_4$@Ti-doped ZnO nanocomposite. This nanocomposite was easily separated by applying an external magnetic field due to $NiFe_2O_4$ magnetic nanoparticles coupled with ZnO. The results show N-doped rGO/$NiFe_2O_4$@Ti-doped ZnO nanocomposite has efficient potential for removing dyes from wastewater.

3:15 PM

(EMA-147-2022) Development on doped-$BaTiO_3$ System Ferroelectrics for Electro-thermodynamic Cycle Power Generation

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2. Nagaoka University of Technology, Japan
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5. Sanjo City University, Faculty of Engineering, Japan

Wasted heat regeneration technology will be an important key to solve the global energy issue. For example, in Japan, the waste heat energy generated annually reaches 1 trillion kWh, which is equivalent to the amount of annual power generation. In addition, 76% of this waste heat energy has been reported to be below 200 °C. The seebeck effect is the mainstream of waste heat regeneration technology, but it will be difficult to regenerate all the waste heat energy blow 200 °C with large temperature fluctuations. To solve this problem, there is a power generation method that does not require a spatial temperature difference and can regenerate waste heat by utilizing the change in crystal structure due to the temperature of the ferroelectric substance and the electric field. As for the contents of the experiment, various elements were doped into a $BaTiO_3$-based ferroelectric with a Curie point of 200 °C or less, and ceramics were synthesized and manufactured in the laboratory. In addition, the amount of power generated was measured with a sample, and the mechanism of improving power generation performance by dopants was crystallographically analyzed by XRD and neutron diffraction. [Acknowledgement] A part of this work was supported by the New Energy Industrial Technology Development Organization (NEDO) through advanced research program for Energy and Environmental Technologies.

4:00 PM

(EMA-148-2022) Colossal electrical conductivity anisotropy in graphene / aluminum nitride ceramics

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New wide-band gap semiconductors (SC) for power electronics such as SiC, GaN and diamond allow higher power densities, leading to higher operating temperatures. However, the surrounding materials also undergo a temperature increase, meaning that a parallel effort is needed in SC packaging technologies research. The substrate, which is one of the essential components, is used to electrically insulate the SC from the rest of the system, drain the generated heat and provide a path to connect the SC to the other elements. Aluminium nitride (AlN) is a very attractive material, due to his high thermal conductivity, excellent mechanical properties and high electrical resistivity. It is a perfect candidate to be used as a substrate. A great challenge is to control the electrical properties of AlN while maintaining the high thermal conductivity. The low dimensional carbon based nanomaterial graphene (GNP) is an excellent candidate to tune the electrical properties of AlN. In the present work, we successfully obtained a new graphene aluminum nitride doped ceramic, obtained by spark plasma sintering. The nanocomposite, comprising the added GNP, was revealed to possess a controllable electrical anisotropy.

4:15 PM

(EMA-149-2022) DC lifetime and thermally stimulated depolarization current (TSDC) of $Bi(Zn,Ti)O_3$-$BaTiO_3$ (BZT-BT)

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$Bi(Zn,Ti)O_3$-$BaTiO_3$ (BZT-BT) is a relaxor dielectric with high energy density and high resistivity at elevated temperatures. Little is known of the long-term stability under high electric fields and elevated temperature of operation for BZT-BT. In this presentation DC lifetime results for BZT-BT with acceptor and donor doping are discussed. The DC lifetime results are correlated with thermally stimulated depolarization (TSDC), impedance spectroscopy, capacitance, and phase and microstructure. Relationships between electrical properties and electronic and ionic defects will be discussed.

4:30 PM

(EMA-150-2022) Mechanical characterization of thin brittle substrates for microelectronic applications

M. Gruber*[1]; P. Supancic[1]; I. Kraleva[1]; R. Bermejo[1]

1. University of Leoben, Institute of Structural and Functional Ceramics, Austria

Materials such as ceramics, glasses or single crystals have found a wide application in microelectronics due to their often unique combination of functional as well as mechanical properties. Nevertheless, the inherent brittle character can limit their applicability whenever those materials are exposed to significant tensile stresses. Those stresses are often inevitable during manufacturing of microelectronic components associated with the different material classes combined, having distinct thermo-mechanical properties. In addition, external loading in service has to be taken into account for reliability assessments, which often rely on results from mechanical testing of bulk (thick) samples. In this work, we develop testing protocols for several thin substrates and components for the microelectronic industry under different loading conditions. A combination of uniaxial and biaxial testing methods (4-point

bending, Ball-on-three-balls and Ring-on-ring testing) for thin substrate materials (glasses; single crystals; low-temperature co-fired ceramics) together with fractographic analyses are proposed, to fully characterize the fracture behaviour of thin brittle microelectronic materials and components. Recommendations on the limitations of the testing methods are also discussed.

4:45 PM

(EMA-151-2022) Investigation of mechanical and electrical properties of lead-free piezoelectric 0-3 composites

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2. Nagoya Institute of Technology, Graduate School of Eng., Dept. Mater. Sci. & Eng., Japan

Mechanical energy can be harvested via the piezoelectric effect, which describes the ability of a material to transduce mechanical into electrical energy, and vice versa. This characteristic is used in several applications, such as the stabilization of "smart" wind turbine blades, or impact-based energy harvesting, etc. In these situations, the piezoelectric device requires increased mechanical stability to ensure a long and reliable life time. To increase the mechanical properties of piezoelectric ceramics, 0-3 composites are generally one way to go. However, the piezoelectric properties decreases significantly and by extension the energy conversion. Interestingly, Seo et. al in 2014, used ZrO_2 as an inclusion in lead-zirconate-titanate, and achieved increased electromechanical properties while increasing the fracture toughness. However, no further research has been conducted in this direction, and the question remains if a similar feat could be achieved with lead-free alternatives. As such, this presentation will elucidate on the underlying mechanisms, as well as give an outlook on future approaches of this concept.

5:00 PM

(EMA-152-2022) Examination of Electrical Properties of Foam Insulators.

I. Gunes*[1]

1. Istanbul University Cerrahpasa, Engineering Faculty, Electrical Engineering Department, Turkey

In this study, the electrical breakdown machined foam insulators. In this paper conductors, insulators, types, electrical characteristics, foam foam insulators and electrical properties of insulators, were informed about the preparation and application areas. Theoretical calculation of the dielectricconstant of the foam are examples of insulators. Provides information about the chemical and physical properties of the foam insulators. Examination of Electrical Properties of Foam Insulators. Especially in recent years, lightness, cheapness and less raw material consumption are prominent in all production sectors. is on the plan. In addition to these features, high impact resistance, increased toughness, increased thermal Polymer-based foam that can also provide properties such as stability, reduced electrical and thermal insulation The use of materials is increasing rapidly. Because of these advantages, it is often used in the industry. Polymers such as polyethylene, poly-urethane, poly-vinyl-chloride and poly-propylene began to be used. An insulator (dielectric) is an electric current without free electrons capable of carrying an electric current.

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

Magnetic, Ferroelectric, and Multiferroic Films and Ceramics

Room: Magnolia A
Session Chair: John Heron, University of Michigan

10:00 AM

(EMA-105-2022) Improper ferroelectricity in ultrathin films (Invited)

J. Nordlander*[1]

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The secondary nature of polarization in improper ferroelectrics is known to promote functional properties beyond those expected for conventional ferroelectrics. For example, in the improper ferroelectric hexagonal manganites, the non-ferroelectric distortive origin of electric polarization enables topologically protected ferroelectric vortex domain patterns, conducting domain walls and multiferroicity. In technologically relevant ultrathin films, however, the improper ferroelectric behavior remains significantly less explored. Here, we discuss the emergence of the coupled improper polarization and primary distortive order parameter in thin films of hexagonal $YMnO_3$. Combining state-of-the-art in-situ optical second harmonic generation and transmission electron microscopy, we separately address the improper ferroelectric state and its distortive driving force. We reveal a pronounced thickness dependence of the improper polarization, which we show originates from the strong modification of the primary order at epitaxial interfaces. Nanoscale confinement effects on the primary order parameter reduce the temperature of the phase transition, which we exploit to visualize its order-disorder character with atomic resolution. Our results thus advance the understanding of the evolution of improper ferroelectricity within the confinement of ultrathin films, which is essential for their successful implementation in nanoscale applications.

10:30 AM

(EMA-106-2022) Controlling charged domain walls with electric fields in h-$YMnO_3$ thin films

A. Bortis*[1]; M. Trassin[1]; M. Fiebig[1]; T. Lottermoser[1]

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Using phase-field simulations, we show how an electric field can be used to deterministically create and destroy charged domain walls in h-$YMnO_3$ thin films. The polarization is driven by a non-polar structural distortion called trimerization. This improper polarization allows for stable charged domain walls. In thin films, previous experiments showed that the trimerization is suppressed because of the lattice mismatch of the film and the substrate. Using Landau theory we model a epitaxial h-$YMnO_3$ system in the ultrathin regime. The suppression of the trimerization at the substrate interface leads to a decrease in the polarization as well as a to a weaker coupling of the polarization to the trimerization, lowering the switching barrier of the polarization at the substrate interface. This enables an uncommon switching mechanism, where instead of random nucleation, ferroelectric domains are only nucleated at the substrate interface, which creates charged domain walls in the film. Therefore, we can use an electric field to tune the density of charged walls in the film. In addition, the suppressed polarization at the interface also reduces the coercive field of the film. This combination of increased density of charged walls and reduced coercivity offers an avenue for implementing low-energy consuming logic devices using improper ferroelectrics.

10:45 AM

(EMA-107-2022) Influence of Varied Sapphire Substrate Topographies on the Multiferroic Properties of Aurivillius Phase Thin Films

L. Colfer*[2]; N. Bagués[1]; M. Bansal[3]; M. Schmidt[4]; B. Long[5]; T. Maity[3]; D. W. McComb[1]; L. Keeney[2]

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2. Tyndall National Institute, University College Cork, Advanced Materials and Surfaces Group, Ireland
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5. University College Cork, School of Chemistry, Ireland

Aurivillius phase, $Bi_6Ti_xFe_yMn_zO_{18}$ (B6TFMO), is a rare example of a room temperature (RT) magnetoelectric multiferroic, demonstrating potential for future application in memory storage devices. Previous reports indicate partitioning of magnetic Mn/Fe cations toward central perovskite (PK) layers of B6TFMO is critical to B6TFMO's RT magnetic response. Stacking fault and out-of-phase boundary (OPB) defects within the layered-type structures can further affect relative proportions of magnetic cations within the PK layers and influence the formation of charged domain walls and unusual polar vortexes. In this work we use sapphire substrates with differing surface topographies to deliberately encourage structural defects in B6TFMO thin films to investigate their impact on ferroelectric (FE) and ferromagnetic (FM) properties. B6TFMO films were deposited by direct liquid injection chemical vapour deposition on miscut and patterned sapphire. Through x-ray diffraction, scanning transmission electron microscopy, energy dispersive x-ray analysis and electron energy loss spectroscopy, the structural and chemical characteristics of our films were examined and the influence of substrate surfaces on defect promotion is considered. The FM and FE properties are discussed through piezoresponse force microscopy and superconducting quantum interference device magnetometry measurements.

11:00 AM

(EMA-108-2022) Layer-by-layer symmetry probing of Aurivillius $Bi_5FeTi_3O_{15}$ thin films by in-situ second harmonic generation

I. Efe*[1]; E. Gradauskaite[1]; M. Fiebig[1]; M. Trassin[1]

1. ETH Zurich, Department of Materials, Switzerland

The highly anisotropic nature of layered oxides brings exotic functionalities such as superconductivity, magnetoresistance and ferroelectricity, which are promising for applications. However, their integration in epitaxial design is challenging due to the complexity of the unit cell, which makes the precise monitoring of the growth a necessity. Reflection High Energy Electron Diffraction (RHEED) is an effective technique to monitor the growth of individual layers, yet it lacks the information on inversion symmetry breaking in the material, which is a key for the functionalities. Here, taking a layered ferroelectric material $Bi_5FeTi_3O_{15}$ as a model system, we use in-situ optical second harmonic generation (ISHG) in combination with RHEED to access the symmetry of our films during the epitaxial deposition process with sub-unit cell accuracy. We identify an oscillating intensity of the ISHG signal during the growth. Using complementary in-situ RHEED and ex-situ atomic force microscopy, we correlate the ISHG oscillations with the surface symmetry evolution of films and the sub-unit-cell stacking evolution during the two-dimensional layer-by-layer growth. Our unique ability to access the symmetry of the films during deposition brings new insights in the design of layered oxide films and new degrees of freedom for the development of energy efficient oxide electronics.

11:15 AM

(EMA-109-2022) Probing the Dynamics of Charged Multiferroic Topologies at the Atomic Scale (Invited)

M. Conroy*[1]; E. O'Connell[2]; S. Griffin[5]; L. Jones[4]; R. Whatmore[1]; K. Moore[3]; C. Downing[4]; U. Bangert[3]; C. Ophus[5]

1. Imperial College London, Materials, United Kingdom
2. Max Planck Institute for the Science of Light & Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany
3. University of Limerick, Physics, Ireland
4. Trinity College Dublin, Ireland
5. Molecular Foundry, Lawrence Berkeley National Laboratory, USA

The complex internal structure, functional properties and dynamic nature of polar topologies in multiferroic oxides offers a rich landscape for materials science research. As the spatial scale of these entities are often sub-atomic in nature and dynamic, time-resolved aberration corrected scanning transmission electron microscopy (STEM) is the ideal characterisation technique. Recently there has been a surge in interest of electron beam based atom by atom manipulation. This presentation will focus on using the applied electric field of a STEM probe to move multiferroic topologies, and thus investigate their dynamics while imaging at the subatomic scale. Using a segmented STEM detector any changes in deflection and thus the changes in polarisation for each domain, can also be investigated with controlled variants in applied field conditions. This allows one to study the influence of different domain patterns on the dynamics of their topologies. By controlling the incoming STEM probe direction, parallel domain walls could be moved around to form stable four-fold charged junctions, thus switching from a neutral to charged state. Then in each frame by quantifying the atomic displacement per unit cell using the open source python based TopoTEM software module, the local polarisation at these charged topological can also be monitored.

11:45 AM

(EMA-110-2022) Non-invasive probing of complex order in ferroelectric|dielectric superlattices

N. Strkalj*[1]; A. Bortis[2]; M. Bernet[2]; J. Bang[2]; M. F. Sarott[2]; M. Campanini[3]; M. Rossell[3]; T. Weber[2]; M. Trassin[2]; M. Fiebig[2]

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3. EMPA, Switzerland

In ferroelectricjdielectric $PbTiO_3|SrTiO_3$ (PTO|STO) superlattices, energy contributions of strain and electrostatics are in a delicate balance, which leads to the stabilization of complex phases. Some of these new states of matter exhibit local negative permittivity and thus have a high potential for energy-efficient electronic devices. Identifying the presence of complex phases is however challenging because of the ordering of dipole moments along multiple axes. We focus on studying the complex order in PTO|STO superlattices using non-invasive methods. Using a non-linear optical approach, second harmonic generation, we first identify the phase coexistence of the ordered multi-domain phase with in-plane polarization and the vortex phase. We furthermore detect interlayer coupling between ferroelectric layers leading to an antiparallel alignment of local polarization in neighboring layers. We then investigate the stabilization and manipulation of in-plane polarization using a combination of x-ray diffraction and piezoresponse force microscopy. Finally, we undergo an in-depth structural analysis of x-ray diffuse scattering to achieve an understanding of the local structure on the atomic level. Our findings pave the way towards using non-invasive techniques for monitoring the evolution of the complex order operando.

12:00 PM

(EMA-111-2022) Deterministic control of ferroelectric polarization by ultrafast laser pulses (Invited)

P. Chen*[1]; C. Paillard[2]; H. Zhao[4]; J. Íñiguez[3]; L. Bellaiche[1]

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4. Jilin University, International Center for Computational Method and Software (ICCMS), China

Ultrafast light-matter interactions present a promising route to control ferroelectric polarization at room temperature, which is an exciting idea for designing novel ferroelectric-based devices. One emergent light-induced technique for controlling polarization consists in anharmonically driving a high-frequency phonon mode through its coupling to the polarization. A step towards such control has been recently accomplished, but the polarization has been reported to be only partially reversed and for a short lapse of time. Such transient partial reversal is not currently understood, and it is presently unclear if a full control of a polarization, by, e.g., fully reversing it or even making it adopt different directions (thus inducing structural phase transitions), can be achieved by activating the high-frequency phonon mode via terahertz pulse stimuli. Here, by means of realistic simulations of a prototypical ferroelectric, we reveal and explain (1) why a transient partial reversal has been observed, and (2) how to deterministically control the ferroelectric polarization thanks to these stimuli. Such results can provide guidance for realizing original ultrafast optoferroic devices.

Ferroelectric Alloys and Ferroelectric Domains I

Room: Magnolia A
Session Chair: Morgan Trassin

2:00 PM

(EMA-153-2022) Wake-up, Retention, and Fatigue in AlN-based Ferroelectrics (Invited)

W. Zhu[1]; J. Hayden[2]; F. He[1]; J. Yang[1]; J. Maria[1]; S. Trolier-McKinstry*[1]

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Polarization reversal is demonstrated in Sc- or B-doped, and undoped AlN films. Between R.T. and 300°C, the coercive field drops by ~50%, while there was small temperature dependence of the remanent polarization. Applying intrinsic/homogeneous switching models produce non-physical fits, while models based on thermal activation suggests that switching is regulated by a distribution of pinning sites or nucleation barriers with an average activation energy near 28 meV. Many of these films undergo wake-up, in which the remanent polarization rises from ~0 $\mu C/cm^2$ to >100 $\mu C/cm^2$. As it does so, the reversible and irreversible Rayleigh coefficients increase, suggesting that the concentration of mobile interfaces is increasing. The irreversible Rayleigh coefficient is ~3.5×10^{-4} cm/kV, four to five orders of magnitude below those of $PbZr_{0.52}Ti_{0.48}O_3$, consistent with the high coercive fields observed in the nitride ferroelectrics. On cycling at 6MV/cm 100Hz, metal – ferroelectric – metal structures first underwent wake-up, then polarization saturation, then a gradual inflation of the apparent remanent polarization due to increases in leakage. After 9.5×10^4 cycles, the apparent polarization decreases due to progressive thermal dielectric breakdown events concentrated near the electrode perimeter. Films also show excellent retention of memory states for hundreds of hours at bake temperatures as high as 200°C.

2:30 PM

(EMA-154-2022) Robust Ferroelectricity in Wurtzite (Zn,Mg)O Thin Films

G. Ryu*[3]; L. Jacques[2]; S. Shetty[1]; S. Trolier-McKinstry[3]; J. Maria[3]

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3-dimensional ferroelectric microelectronics (3DFeM) have attracted attention due to the promise of substantial reductions in the energy cost of computation. However, scaling has stalled with perovskite-type ferroelectric thin films due to high processing temperature and strong thickness-dependence to the functional properties. To overcome this challenge, we has developed the wurtzite (1-x)ZnO-xMgO ($x = 0 \sim 0.40$) epitaxial thin films via a radio frequency magnetron co-sputtering. The films showed smooth surfaces and interfaces and uniform distribution of cations across the films. Robust remanent polarizations (60 ~ 120 $\mu C/cm^2$) were obtained in the wide range of Mg concentration following a wake-up process. Polarization hysteresis loops exhibited a strong temperature-dependence for ferroelectric switching. While the remanent polarizations increased minimally with temperature, coercive electric fields significantly decreased from ~2.5 MV/cm to ~1.5 MV/cm with ~35 meV of pseudo-activation energy. This presentation will highlight the structure-processing-property relationships in ZnO-MgO films with attention to the importance of synthesis conditions including bombardment, working gas pressure, target conditioning, and flux ratios. Special attention will be given to exploring the wake-up process and discussing a model based on interfacial nuclei formation that seed the polarization reversal process.

2:45 PM

(EMA-155-2022) Impact of Oxygen Content on Crystallization and Ferroelectric Behavior of Hafnium Oxide Thin Films

S. T. Jaszewski*[1]; E. Hogland[1]; A. Costine[1]; M. Weber[3]; S. Fields[2]; M. T. Sales[1]; J. Vaidya[4]; L. Bellcase[6]; K. Loughlin[6]; A. Salanova[2]; M. D. Henry[5]; J. Maria[7]; J. L. Jones[6]; N. Shukla[4]; S. McDonnell[1]; P. Reinke[1]; J. Ihlefeld[2]

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5. Sandia National Laboratories, USA
6. North Carolina State University, Dept. of Materials Science & Engineering, USA
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The impact of O_2 content in the plasma during High Power Impulse Magnetron Sputtering on the crystallization and ferroelectric properties of HfO_2 films is investigated. 20 nm HfO_2 films were sputtered from a 99.9% purity Hf metal target in Ar/O_2 atmosphere with varying O_2 content. Grazing-incidence XRD measurements showed that films with the lowest and intermediate O_2 content resulted in orthorhombic and/or tetragonal phases, while those with the highest O_2 content resulted in monoclinic phase. These differences in phase constitution resulted in unique polarization responses. Grain size measurements revealed equivalent microstructures for each film, suggesting that oxygen content, and not microstructure, is a significant contributor to phase stability. Oxygen content in the films was measured before and after rapid thermal annealing using XPS, and showed an increase in the oxygen/hafnium ratio with an increase in oxygen in the plasma, with values of x in HfO_x ranging from 1.3 to 1.7 after annealing. Additionally, differences in the oxygen vacancy concentrations in the films, which correlated with the changing O/Hf ratios, were observed using XPS in conjunction with Electron Energy Loss Spectroscopy and Positron Annihilation Spectroscopy. These results provide evidence that oxygen content has a significant impact on phase stability in ferroelectric HfO_2 films.

3:00 PM

(EMA-156-2022) Rhombohedral $Hf_{0.5}Zr_{0.5}O_2$ thin films: Ferroelectricity and devices (Invited)

Y. Wei*[1]; P. Nukala[2]; B. Noheda[3]

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2. Indian Institute of Science, India
3. University of Groningen, Netherlands

The ferroelectricity found in the simple oxide doped-HfO_2 thin films, brought a big surprise to the ferroelectrics community. This novel material could potentially solve most of the roadblocks in the way to a ferroelectric memory. From the fundamental point of view, it also appeals to many researchers interested in understanding the origin of ferroelectricity in this material, which in turn could give insights to improve device properties for applications. Here, we will introduce the development of epitaxial high-quality $Hf_{0.5}Zr_{0.5}O_2$ (HZO) thin films, which show a new (rhombohedral) phase different from the usually reported orthorhombic one. In addition, a systematic study was conducted to offer a guideline to stabilize this ferroelectric phase. The epitaxial nature of HZO thin films on $La_{0.7}Sr_{0.3}MnO_3$ electrodes allows for an in-depth microstructural investigation of the switching mechanisms in hafnia-based devices. Furthermore, taking advantage of the ferromagnetic electrodes in our heterostructures, hafnia-based multiferroic tunnel junctions were fabricated and studied.

Ferroelectric Alloys and Ferroelectric Domains II

Room: Magnolia A
Session Chair: Morgan Trassin

4:00 PM

(EMA-157-2022) Preparation of Ta-Substituted ZrO_2 Films for Ferroelectric Memory Devices

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Ferroelectric HfO_2-based films are considered to be a candidate for highly integrated ferroelectric memory devices such as FeFETs because these materials have Si and CMOS compatibility and low required processing temperatures appropriate for BEOL integration. Common HfO_2 based films comprise an orthorhombic ($Pca2_1$) phase and have remanent polarization (P_r) ~ 20 μC/cm^2. FeFETs require less than 10 μC/cm^2 to prevent large charging and dielectric breakdown ferroelectric layer of the linear dielectric interlayer. Therefore, the development of a novel CMOS compatible ferroelectric with low P_r is required. Here, we focus on Ta substituted ZrO_2, which has a reported wide composition range of $Pca2_1$ phase stability with different lattice constant from HfO_2, and study the control of lattice constant and polarization using this material. Our calculations from previous crystallographic data reveal a 40% reduction in the spontaneous polarization (P_s) compared to HfO_2. We will report the preparation of Ta substituted ZrO_2 films by pulsed laser deposition and chemical solution deposition, and its crystal structure and electrical properties and will show clear evidence of ferroelectric stability and response.

4:15 PM

(EMA-158-2022) Multilevel polarization switching in ferroelectric thin films

M. F. Sarott*[1]; M. Rossell[2]; M. Fiebig[1]; M. Trassin[1]

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The ever-increasing interest in materials for memristive and neuromorphic applications showing non-discrete responses calls for a paradigm shift from intrinsically binary ferroics towards continuously tunable ferroic states. In this work, we demonstrate that we can arbitrarily set the magnitude of the remanent ferroelectric polarization at the nanoscale in epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ thin films with a single DC bias. By driving the ferroelectric system towards an instability near the PZT morphotropic phase boundary and controlling the resulting softness via epitaxial strain, we favor the formation of decoupled nanometric 180° domains that exhibit a broad coercive field distribution. Using in-situ optical second harmonic generation and X-ray diffraction, we investigate the emergence of the nanoscopic domain configuration. We then use piezoresponse force microscopy to reveal a multilevel switching capacity that reversibly enables accessing any remanent state between non-polar and fully saturated. Ultimately, to highlight the direct technological relevance of non-binary polarization switching, we demonstrating a quasi-continuous tunability of the tunnel electroresistance and the non-linear optical response.

4:30 PM

(EMA-159-2022) Electrostatic effects in nanoscale ferroelectrics (Invited)

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The behavior of nanoscale forms of matter, such as thin films or nanocrystal, is strongly influenced by the structure and behavior of their surfaces and interfaces. In nanoscale ferroelectrics, a surface charge arises as a consequence of the ferroelectric polarization itself, and this surface charge leads to an electrostatic instability - the so-called "polar catastrophe" - if it is not compensated. Here we show how the properties of ferroelectric materials at the nanoscale are intimately linked to the compensation mechanism that takes place at their surface. We also demonstrate how the structural and electronic properties of $PbTiO_3$, $BiFeO_3$ and $KTaO_3$ lead to a different compensation mechanism in each case, and we discuss how to harness the properties of these nanoscale materials for technological applications.

5:00 PM

(EMA-160-2022) Natural limits to minimum domain size in barium titanate using multi-scale modeling

A. J. Klomp*[1]; R. Khachaturyan[2]; T. Wallis[2]; A. Grünebohm[2]; K. Albe[3]

1. TU Darmstadt, Materials Science, Germany
2. Ruhr-Universität Bochum, ICAMS, Germany
3. Technical University Darmstadt, Fachgebiet Materialmodellierung, Germany

Properties of materials and devices that rely on ferroelectric (FE) properties are often governed by the behavior of FE domain walls (DWs) that separate regions of different polarization orientation. In application such as FE memory devices the stability of the DW structure itself becomes the determining functional property. Naturally, the question arises if there is a lower limit to domain size or the spacing between domain walls. We address this topic using a multi-scale modeling approach in the model FE barium titanate (BT). With a focus on T180 DW we reveal that below a certain size domains spontaneously collapse and merge into larger domains. This observation is independent of atomistic details and is congruent between atomistic and effective Hamiltonian modeling approaches. The size limit is strongly temperature dependent. Besides a phenomenological description of the statistical probability for domain collapse we also relate the different steps of the process to the local energy landscape. As correlation effects are prominent in ferroic materials we, additionally, investigate if and how strong correlations between neighboring DWs can appear. Finally, we extend our investigations to T90 DWs. Despite limitations due to strained DWs we find a similar behavior for this DW type which has been shown to be very relevant to switching processes in BT.

5:15 PM

(EMA-161-2022) Tunable microwave conductance of nanodomains in ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ thin film

S. R. Burns*[1]; A. Tselev[2]; A. Ievlev[3]; J. Agar[4]; L. W. Martin[5]; S. Kalinin[3]; D. Sando[6]; P. Maksymovych[3]

1. University of Calgary, Canada
2. University of Aveiro, Portugal
3. Oak Ridge National Lab, USA
4. Lehigh University, USA
5. University of California, Berkeley, Materials Science and Engineering, USA
6. University of New South Wales, Australia

Ferroelectric materials exhibit spontaneous polarization that can be switched by electric field. Beyond traditional applications as non-volatile capacitive elements, the interplay between polarization and electronic transport in ferroelectric thin films has enabled a path to neuromorphic device applications involving resistive switching. A fundamental challenge is that finite electronic conductivity may introduce considerable power dissipation and perhaps destabilize ferroelectricity itself. Here, we reveal tunable microwave frequency electronic response of domain walls injected into ferroelectric lead zirconate titanate ($PbZr_{0.2}Ti_{0.8}O_3$, PZT) on the level of a single nanodomain. We detected tunable microwave response through first-order reversal curve spectroscopy combined with scanning microwave impedance microscopy (sMIM) measurements. We have investigated contributions of film interfaces to the measured ac conduction through subtractive milling. Using statistical analysis and finite element modelling, we inferred that the mechanism of tunable microwave conductance is the variable area of the domain wall in the switching volume. These observations open the possibilities for ferroelectric memristors, localized to several tens of nanometres and operating according to well-defined dynamics under an applied field.

5:30 PM

(EMA-162-2022) Oxygen vacancy injection as a pathway to enhancing electromechanical response in ferroelectrics

K. Kelley*[1]; A. Morozovska[2]; E. Eliseev[2]; V. Sharma[3]; D. E. Yilmaz[4]; A. C. van Duin[4]; P. Ganesh[1]; A. Borisevich[1]; S. Jesse[1]; P. Maksymovych[1]; N. Balke[1]; S. Kalinin[1]; R. Vasudevan[1]

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2. National Academy of Science Ukraine, Ukraine
3. Oak Ridge National Lab, USA
4. Pennsylvania State University, USA

In ferroelectric systems, the static properties of defects such as oxygen vacancies are well explored, but the dynamic effects are less understood. Here, we utilize piezoresponse force microscopy (PFM) to demonstrate that coupling between bulk electrochemistry and polarization dynamics can yield enhanced electromechanical responses in $BaTiO_3$ thin films. We posit that a local increase in oxygen vacancy concentration under the PFM probe during biasing results in an enhanced electromechanical response due to a created internal electric field that further activates the intrinsic electrostriction. Our arguments are supported by temperature dependent band excitation PFM in ultra-high vacuum (2E-10 Torr), scanning transmission electron microscopy (STEM), and a combination of modeling techniques including finite element modeling, Reactive Force Field (ReaxFF), and Density Functional Theory calculations. Collectively, experimental and theoretical observations point towards the discovery of a new method of enhancing functional responses (Tc, piezo-strain) in ferroelectrics, that has considerable implications for the field both in terms of fundamental understanding of what drives high piezoelectric response, as well as how to better design materials with superior electromechanical properties.

S4: Complex Oxide Thin Films and Heterostructures: From Synthesis to Strain/ Interface-engineered Emergent Properties

Controlled Synthesis of Lateral and Vertical Heteroepitaxial Thin Films and Nanocomposites II

Room: Orange A

Session Chair: Xia Hong, University of Nebraska-Lincoln

10:00 AM

(EMA-112-2022) Stabilizing Otherwise Unstable Complex Oxides through Tailored Superlattices (Invited)

L. Wang*[1]

1. Pacific Northwest National Laboratory, USA

Recent discovery of superconductivity in $Nd_{0.8}Sr_{0.2}NiO_2$ motivates the synthesis of other nickelates for providing previously unknown insights into the origin of high-temperature superconductivity. However, the synthesis of stoichiometric $R_{1-x}Sr_xNiO_3$ thin films over a range of x has proven challenging. Moreover, little is known about the structures and properties of the end member $SrNiO_3$. Here, we show that spontaneous phase segregation occurs while depositing $SrNiO_3$ thin films on perovskite oxide substrates by molecular beam epitaxy. Two co-existing oxygen-deficient Ruddlesden-Popper (RP) phases, Sr_2NiO_3 and $SrNi_2O_3$, are formed to balance the stoichiometry and stabilize the energetically preferred Ni^{2+} cation. On the other hand, by epitaxially synthesizing a set of $(SrNiO_3)_1/(LaFeO_3)_n$ superlattices, we show that perovskite $SrNiO_3$ can be stabilized. Spectroscopy reveals that the n = 1 superlattice contains Ni^{3+} and Fe^{4+}, whereas Ni^{4+} and Fe^{3+} are observed in the n = 5 superlattice. Our DFT calculation results show that the B-site cation valences can be tuned by controlling the magnitude of the FeO_6 octahedral rotations, which in turn drive the energy balance between Ni^{3+}/Fe^{4+} and Ni^{4+}/Fe^{3+}, thus controlling emergent electrical properties.

10:30 AM

(EMA-113-2022) Synthesis of an immiscible epitaxial oxide heterostructure with tunable wavelength-selectivity

M. Webb*[1]; S. McSherry[2]; J. Kaufman[3]; Z. Deng[1]; T. Ma[4]; E. Kioupakis[1]; K. Esfarjani[3]; A. Lenert[2]; J. Heron[1]

1. University of Michigan, Materials Science and Engineering, USA
2. University of Michigan, Chemical Engineering, USA
3. University of Virginia, USA
4. University of Michigan, Michigan Center for Materials Characterization, USA

Thermal emitters with wavelength-selective optical properties derived from alternating materials with refractive index contrast are of interest in applications of energy conversion, sensing, imaging, and thermoregulation. Thermal emitters with extrinsically designed optical properties, however, suffer from poor thermal stability at elevated temperature (>1000 °C). Here, we demonstrate a tunable, and wavelength-selective oxide heterostructure made from alternating layers of $BaZr_{0.5}Hf_{0.5}O_3$ (n = 2.2) and MgO (n = 1.7), capable of suppressing undesired thermal emission at a desired cutoff wavelength. The heterostructure exhibits coherent atomic registry that retains clearly separated refractive index mismatched layers without interface coarsening, interdiffusion, phase change, or decomposition up to 1100 °C in dry air. The use of dissimilar crystal structures, with low lattice and thermal expansion mismatch, allows for high crystallinity superlattices with interlayer immiscibility at high temperature. The understanding gained from this study can be used to develop thermally stable and wavelength selective emitters for thermophotovoltaic applications. [Distribution Statement "A" (Approved for Public Release, Distribution Unlimited)]

10:45 AM

(EMA-114-2022) Exsolution synthesis of tunable multifunctional thin-film nanocomposite

J. Wang*[1]; K. Syed[2]; S. Ning[1]; I. Waluyo[3]; A. Hunt[3]; E. Crumlin[4]; A. K. Opitz[5]; C. Ross[1]; W. Bowman[2]; B. Yildiz[1]

1. Massachusetts Institute of Technology, USA
2. University of California, Irvine, Department of Materials Science & Engineering, USA
3. Brookhaven National Laboratory, USA
4. Advanced Light Source, USA
5. TU Wien, Institute of Chemical Technologies and Analytics, Austria

Next-generation electrochemical and electronic devices require scalable synthesis methods to fabricate multi-functional thin-film nanocomposites. Exsolution is a partial decomposition process where metallic nanoparticles are precipitated out of the host metal-oxide matrix upon reduction. While exsolution has been extensively employed to enhance surface catalytic properties in a broad range of applications, its potential to modulate bulk properties remains open. Using thin-film $La_{0.6}Sr_{0.4}FeO_3$ (LSF) as a model system, we show the novel utility of exsolution in fabricating self-assembled metal oxide nanocomposites with tunable functionalities. Combining multi-modal characterization with numerical modeling, we assessed the chemical, magnetic, and electrical properties of the exsolution-synthesized nanocomposite at different stages of Fe^0 exsolution as well as during redox cycling. Upon exsolution, we observed an increase in the electronic conductivity by more than two orders of magnitude, turning LSF from a dominantly ionic conductor to a dominantly electronic conductor. Moreover, the exsolved nanocomposite is redox-active even at moderate temperatures, enabling a continuous modulation of magnetization between 0 and 110 emu/cm^3. These findings point out that exsolution may serve as a platform for scalable fabrication of complex metal oxide nanocomposites for electrochemical and electronic applications.

11:00 AM

(EMA-115-2022) Ordered Hybrid Metamaterial of $La_{0.7}Sr_{0.3}MnO_3$-Au Vertically Aligned Nanocomposites Achieved on Templated $SrTiO_3$ Substrate

J. Lu*[1]; R. Paldi[1]; Y. Pachaury[1]; D. Zhang[1]; H. Wang[1]; M. Kalaswad[1]; X. Sun[1]; J. Liu[1]; X. Phuah[1]; X. Zhang[1]; A. El-Azab[1]; H. Wang[1]

1. Purdue University, School of Materials Engineering, USA

Coupled multifunctionalities in nanocomposite thin films offer a pathway toward future integration of device applications. The oxide–metal two-phase nanocomposite thin films in a vertically aligned nanocomposite (VAN) morphology allow for unique structural control and functionality tuning toward future nanoscale devices. However, achieving in-plane ordering of the two phases remains challenging. In this work, we demonstrate an initial success of in-plane long-range ordering achieved in a new oxide–metal VAN system, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO)–Au, through annealed $SrTiO_3$ (STO) substrates. The combination of plasmonic Au and ferromagnetic LSMO enables multifunctionalities, including magneto-optic coupling, hyperbolic dispersion, and tunable ferromagnetic anisotropy. Beyond this LSMO–Au VAN system demonstrated in this work, the long-range ordered two-phase structures induced by perovskite substrate surface terraces can be applied to other oxide–metal VAN systems.

11:15 AM

(EMA-116-2022) Oxygen Transfer in Oxide Heterostructures

K. Kang[2]; A. Chen*[1]

1. Los Alamos National Lab, USA
2. Kyungpook National University, Republic of Korea

Oxygen transfer exists between film and substrate during thin film synthesis. Such a character is extremely critical to control the growth of some metastable phases and understand emergent phenomena at heterointerfaces. By using such an oxygen transfer, we propose a method of controlling the oxygen content of films by engineering the substrate before the growth. The oxide substrate serves as an oxygen sponge, which provides a tunable oxygen environment ranging from oxygen-rich to oxygen-poor for the film growth, depending on the pre-substrate annealing (PSA) conditions. Using manganite as a model system, we demonstrate that this simple PSA method leads to remarkable changes in the structure and physical properties of the as-grown films. In addition, it was found that the oxygen transfer is strongly tied to the oxygen condition in the as-grown oxide layer. The oxygen transfer effect, can be applied to explore not only emergent interfacial phenomena but also the growth of a variety of functional oxide thin films and nanocomposites to tune oxygen content and functional properties.

Strain- and Interface-controlled Device Performance

Room: Orange A

Session Chair: Ambrose Seo, University of Kentucky

2:00 PM

(EMA-163-2022) Engineering iridate superlattices for capturing and controlling antiferromagnetic fluctuations (Invited)

J. Liu*[1]

1. University of Tennessee, USA

Increasing attention has been paid to correlated oxides with strong spin-orbit coupling (SOC), especially those hosting 4d and 5d electrons. A prominent example is the square-lattice iridates due to remarkable similarities to weakly spin-orbit-coupled high-Tc cuprates. This analogy points to an intriguing SOC-correlation interplay, which remains elusive because of the limited number of available bulk compounds. This material bottleneck can be overcome by epitaxial synthesis of artificial pseudospin-half square lattices at the limit of quantum confinement. In this talk, I will discuss our recent work on perovskite (SrIrO3)n/(SrTiO3)m superlattices, which are designed not only to replicate the magnetic state and excitations but also afford excellent tunabilities beyond the Ruddlesden-Popper phases. By resonant x-ray scattering, we demonstrated control of the antiferromagnetic structure by epitaxially implanting structural modulations, which further enables giant responses of the 2D antiferromagnetic fluctuations to uniform magnetic field. Significant magnetoresistance above the Neel temperature is also observed due to spin-charge fluctuations that are characteristic of the Slater-Mott crossover. We are able to tune the system within the crossover by epitaxial strain and gating. The results showcase the rich emergent behaviors and functional properties beyond the analogy with cuprates.

2:30 PM

(EMA-164-2022) Perpendicular Magnetic Anisotropy and Magnetotransport Anomaly in Ultrathin Ferrimagnetic Spinel $NiCo_2O_4$ (Invited)

X. Hong*[1]

1. University of Nebraska-Lincoln, Physics and Astronomy, USA

The high Curie temperature and high spin polarization of the inverse spinel ferrimagnetic $NiCo_2O_4$ make it a promising material candidate for spintronic applications. The magnetic state of epitaxial $NiCo_2O_4$ thin films depends sensitively on the strain and disorder effects, which can lead to unconventional spin transport properties. In this talk, I will discuss our recent magnetotransport studies of high quality 1.5-30 unit cell $NiCo_2O_4$ films deposited on (001) $MgAl_2O_4$ substrates. The switching hysteresis of anomalous Hall signal shows that out-of-plane magnetic anisotropy is sustained in ultrathin films down to 1.5 unit cell (1.2 nm) thickness. The anomalous Hall resistance shows a nonmonotonic temperature dependence and exhibits a sign reversal driven by both temperature and film thickness. The scaling relation between the anomalous

Hall conductivity and longitudinal conductivity reveals the intricate interplay between the spin-dependent impurity scattering, the band intrinsic Berry curvature, and the correlation effect. Our study provides important materials insights that can facilitate the functional design of $NiCo_2O_4$ films for applications in magnetic sensing and epitaxial magnetic tunnel junctions.

2:45 PM

(EMA-165-2022) Solid-State Electrochemical Control of Physical Properties for Transition Metal Oxide Epitaxial Films with Perovskite-Related Crystal Structures (Invited)

H. Ohta*[1]; Q. Yang[2]; H. Jeen[3]

1. Hokkaido University, Research Institute for Electronic Science, Japan
2. Hokkaido University, Graduate School of Information Science and Technology, Japan
3. Pusan National University, Department of Physics, Republic of Korea

Several transition metal oxides (TMOs) having perovskite-related crystal structures show drastic changes in physical properties accompanied by the oxidation state change in TM ions. For example, strontium cobaltite shows metal to insulator phase transition with the oxidation state change of Co from +4 to +3. Since this phase transition is nonvolatile, we expect that a new type of memory device is realized. Among several ways to control the oxidation state of Co, the electrochemical way is the most promising way. However, the use of ionic liquid or liquid electrolyte is not appropriate for practical application due to the liquid leakage problem. In my talk, I demonstrate solid-state electrochemical control of physical properties for TMO epitaxial films with perovskite-related crystal structures; $SrCoO_x$ and $SrFeO_x$. We used YSZ or mesoporous insulator as the solid electrolyte and successfully controlled the oxidation states of Co or Fe by the electrochemical oxidation/reduction or oxidation/protonation.

3:00 PM

(EMA-166-2022) Strain-Controlled Atomic Scale Distortions and Anti-Ferromagnetism at $LaFeO_3/SrTiO_3$ Interface

M. Zhu*[1]; J. Flores[2]; J. Lanier[2]; S. Polat Genlik[1]; M. Ghazisaeidi[1]; F. Yang[2]; J. Hwang[1]

1. Ohio State University, Material Science and Engineering, USA
2. Ohio State University, Department of Physics, USA

Strain-induced atomic-scale modification of magnetic canting in antiferromagnetic insulator $LaFeO_3$ is studied using scanning transmission electron microscopy. Antiferromagnetic insulators gain attention as next-generation spintronics candidates. Control of magnetic properties via external stimuli, such as strain, is needed for applications. In this study, we observed notable changes in magnetic canting in thin $LaFeO_3$ films (under compressive strain) grown on $SrTiO_3$ substrates. We trace the structural origin of the change in magnetism to the changes in the lattice distortion at the interface. First, the rotation of Fe-O octahedra changes within the first ~6 unit cells, progressively decreases near the interface. Cation (La) positions are also affected by the strain at the interface, showing less distortion due to the connection to the cubic $SrTiO_3$. Nanoscale structural domains with different orientations were also observed, which may have important implications for the formation of magnetic domains near the interface. Based on the experimental results, density functional theory calculation is performed to help elucidate the exact mechanism of the observed structure-property relationship. Our current study, therefore, provides an atomic-level understanding of fast, efficient tuning of the magnetic states that is essential to advancing next-generation spin-electronics.

3:15 PM

(EMA-167-2022) Phase and structural investigation of SrxNbO3 thin films grown via pulsed laser deposition

S. S. Almishal*[1]; G. N. Kotsonis[1]; J. Maria[1]

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

Efficient transparent conducting electrodes with low electrical resistivity remain a substantial need in optoelectronic applications. Sr_xNbO_3 with x<1 have been identified as high-performance conductors with transparency in the visible and ultraviolet regime. In this work, the growth of Sr_xNbO_3 thin films by pulsed laser deposition is investigated. The relationship linking target formulation, synthesis conditions, and substrate crystal structure to the ability to stabilize the perovskite phase is highlighted. X-ray diffraction and atomic force microscopy results will be presented to demonstrate condition/formulation combinations that produce perovskite films and those which promote step-flow growth. Transport properties will be characterized by temperature dependent resistivity analysis. Currently phase pure perovskite films can be produced when Sr:Nb ratios fall within the (0.7-0.95): 1 range -for such materials, room temperature resistivity is in the order of $10^{-5}\Omega$-cm. We will present the results of stability calculations performed using density functional theory to understand how A-site filling fraction influences internal energy trends. Preliminary investigations on introducing configurational entropy onto the B-site will be presented. By substituting a mixture of transition metals on the B-site, it may be possible to tune carrier concentration and conductivity.

Synthesis and Properties of High Entropy Complex Oxides

Room: Orange A
Session Chair: Jian Liu, University of Tennessee

4:00 PM

(EMA-168-2022) Complex Oxide Heterostructures with Controlled One-Dimensionality (Invited)

A. Seo*[1]

1. University of Kentucky, Physics and Astronomy, USA

Tuning the dimensionality of a system offers a tool for realizing new quantum phenomena associated with phase transitions and topological properties. However, only a few naturally occurring complex oxides with tunable, intrinsic one-dimensional (1D) structures are available for experimental studies. In this talk, I will present an approach of synthesizing 1D quantum stripe systems by creating dimensionally confined superlattices from in-plane oriented layered materials. For example, 1D IrO_2 stripes are synthesized using a-axis oriented superlattices of Sr_2IrO_4 and $(La,Sr)GaO_4$, both are of the K_2NiF_4 symmetry. The dimensional confinement of the superlattices has been confirmed by structural characterizations. Optical spectroscopy shows clear anisotropic characteristics and dimensional electronic confinement of the spin-orbit coupled $J_{eff} = 1/2$ band. Spin and orbital excitations observed in resonant inelastic x-ray scattering spectra suggest larger exchange interactions and more confined orbital excitations in the 1D IrO_2 stripes than single crystals. The observed electronic confinement and localized spin structure are quite consistent with density functional theory calculations. This method of synthesizing 1D stripe-superlattices is a viable technique for obtaining dimensionality-induced quantum phase transitions, in which exotic excitations such as the fractional quantizations of quasi-particles can emerge.

4:30 PM

(EMA-169-2022) Thermal and mechanical properties of the entropy stabilized oxide $(MgCoNiCuZn)_{0.2}O$ across the critical temperature

C. M. Rost*[2]; D. Schmuckler[2]; C. Bumgardner[1]; M. Hoque[1]; D. Diercks[4]; G. N. Kotsonis[3]; J. Maria[3]; G. L. Brennecka[6]; X. Li[5]; P. E. Hopkins[1]

1. University of Virginia, Mechanical & Aerospace Engineering, USA
2. James Madison University, Physics and Astronomy, USA
3. Pennsylvania State University, Materials Science and Engineering, USA
4. Colorado School of Mines, Metallurgical and Materials Engineering, USA
5. University of Virginia, USA
6. Colorado School of Mines, USA

Entropy stabilized oxides (ESOs) are a sub-class of high entropy ceramics, unique in that they are shown that their phase stability is driven by configurational entropy—created through mixing equimolar amounts of several binary oxide components to dominate a positive enthalpy of mixing. The nature of this phase change is physically reversible; above a critical temperature the system presents as a single-phase, high symmetry solid solution. Below this temperature is a multi-phase composite, where a secondary phase precipitates from the host. Even with the presence of a secondary phase, the material still exhibits a key characteristic of a high entropy system in that the number of phases present is below predictions from the Gibbs phase rule. As various property studies continue to emerge on high entropy and entropy-stabilized ceramics, we seek further understanding of property changes as we cross the phase boundary between "high-entropy" and "entropy-stabilized". In this talk, we report some of the thermal and mechanical properties of entropy stabilized oxide $(MgCoNiCuZn)_{0.2}O$ across the transition from a multi-component high entropy oxide to a single phase ESO.

4:45 PM

(EMA-170-2022) Impact of Synthesis Conditions on the Local Structure of Entropy Stabilized Oxides

T. Valentine*[1]; C. M. Rost[1]; M. Webb[2]; P. Meisenehimer[2]; J. Heron[2]; C. M. Rost[1]

1. James Madison University, USA
2. University of Michigan, USA

Entropy-stabilized oxides (ESO)s are a unique material class that bypasses the influence of enthalpy in predictable phase formation through a drastic increase of configurational entropy. Although most of the current literature focuses on the application prospects of these ceramics and their potential use in a wide range of technologies, we focus on the fundamental characteristics that ultimately govern their behavior. This study explores the relationship between the synthesis conditions and local structure and chemistry of six- and seven-component ESO thin films grown on MgO. Three compositions were synthesized using pulsed laser deposition: $(CoMgNiCuZnCr)_{0.167}O$, $(CoMgNiCuZnMn)_{0.167}O$, and $(CoMgNiCuZn)_{0.167}(CrMn)_{0.0835}O$ under varying temperatures and pressures. Using X-ray absorption fine structure (XAFS) spectroscopy, we reveal the effect of varying synthesis conditions on element specific averaged local structure, in hopes to strengthen our understanding of the tunability limits of these novel compositions.

5:00 PM

(EMA-171-2022) $Y_{0.2}La_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ Epitaxial Growth and Optical Properties

G. N. Kotsonis*[1]; J. Maria[1]

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

Pr multivalency in the rare earth-based high entropy oxide $Y_{0.2}La_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ (F1) leads to variable oxygen stoichiometry and a tunable optical band gap. F1 takes a fluorite-derived crystal structure with some degree of local bixbyite-type chemical ordering (typical of Y_2O_3), depending on oxygen partial pressure, thermal history, and microstructure. This talk discusses structural and optical trends in F1 thin films grown by laser ablation and RF sputtering. Low partial oxygen pressure during growth or annealing typically results in a larger lattice parameter and optical band gap. Films appear to have fluorite structure and symmetry, contrasting bulk samples, which tend to exhibit bixbyite-type ordering. Tunable oxygen stoichiometry in the F1 system provides opportunities to understand how synthesis conditions can influence cation valence, chemical ordering, and electronic properties in oxygen-deficient high entropy oxide solutions.

5:15 PM

(EMA-172-2022) Configurational Disorder in High Entropy T′ Phase Ruddlesden-Popper Perovskites

D. J. Rossi*[1]; A. R. Mazza[2]; X. Gao[2]; B. Musico[3]; T. Valentine[4]; Z. Kennedy[1]; T. Z. Ward[5]; C. M. Rost[1]

1. James Madison University, Physics and Astronomy, USA
2. Oak Ridge National Lab, Materials Science and Technology, USA
3. University of Tennessee, Materials Science and Engineering, USA
4. James Madison University, USA
5. Oak Ridge National Lab, USA

Recent work has been done to introduce configurational disorder into T' phase Ruddlesden-Popper perovskites using the high entropy approach. An important aspect of understanding how said disorder effects properties is to observe local structural characteristics. Using X-ray absorption fine structure spectroscopy (XAFS), we investigate the local structure of three RP compositions: $(LaPrNdSmEu)_{0.4}CuO_4$, $(LaPrNdSmEu)_{0.34}Ce_{0.15}CuO_4$, and $(LaPrNdSmEu)_{0.32}Sr_{0.2}CuO_4$ thin films grown on strontium titanate. XAFS spectra were taken at Sector 10 of the Advanced Photon Source and analyzed using the Demeter suite of programs. This talk discusses our methodology in understanding the distortions/ local effects resulting from the population of many lanthanide species on a single sublattice, and how these distortions may affect properties such as superconductivity.

S6: Emerging Semiconductors Materials and Interfaces

Control and Characterization over Defects and Dopant

Room: Citrus B

Session Chairs: Yun-Yi Pai, Oak Ridge National Lab; Jaekwang Lee

10:00 AM

(EMA-117-2022) First-principles studies of the energetic and electronic properties of charged defects, dopants, and complexes in 2D materials (Invited)

R. G. Hennig*[1]

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

Two-dimensional (2D) semiconducting materials have attracted extensive research interests for optoelectronics, spintronics, photovoltaics, and catalysis applications. Realizing their potential in such applications requires a good understanding of the effects of defects, dopants, and impurities on the properties of these systems. We perform density functional theory (DFT) calculations to accurately compute formation energies, charge transition levels, and electronic properties of dopants, defects, and complexes in the technologically significant 2D semiconductor materials focusing on the metal chalcogenides MoS_2, WSe_2, SnS, and phosphorene [1-4]. We investigate the dependence of computed defect properties on different levels of theory, utilizing a correction scheme to ensure appropriate electrostatic boundary conditions for charged defects in 2D materials. Some defects induce structural distortions, e.g., Jahn-Teller and other lattice reconstructions, altering electronic properties. We identify dopants that bind with intrinsic defects to form complexes, passivating the dopants and rendering them less effective. Finally,

we demonstrate how theoretical predictions based on DFT and beyond-DFT approaches can help inform the interpretation of experimental results.

10:30 AM

(EMA-118-2022) Impact of Dopants and Film Thickness on the Thermal Conductivity of Indium Phosphide

C. Perez*[1]; D. Taljera[2]; Z. Lui[2]; J. Ryu[2]; D. Botez[2]; V. Gopalan[3]; L. Mawst[2]; B. M. Foley[1]

1. Pennsylvania State University, Mechanical engineering, USA
2. University of Wisconsin Madison, USA
3. Pennsylvania State University, USA

This work presents our measurements of thermal conductivity for bulk and thin film InP materials, with a particular focus on the impact of film thickness and Si dopant concentration in films pertinent to quantum cascade laser (QCL) devices. It is essential to quantify the variation of thermal conductivity as a function of these important design elements and parameters; therefore we conduct time-domain and steady-state thermoreflectance (TDTR, SSTR) measurements over a larger temperature range from 80 – 450 K to understand the dominant phonon scattering mechanisms that impact the thermal conductivity. Insight into these scattering mechanisms' influence is gained through the application of various models based on kinetic theory, called the phonon-gas model. Using this model, we can characterize the relative strength of the point-defect and boundary scattering mechanisms that influence ultimate thermal conductivity in InP-based materials, filling the knowledge gap regarding the thermal properties of materials that are important to QCLs. Overall, this work contributes to the further understanding of the thermal challenges related to materials of interest for advanced QCLs with an ultimate goal of developing innovative solutions for thermal management.

10:45 AM

(EMA-119-2022) Grain and Grain Boundary photoconduction in Perovskite Solar Cells with Tomographic AFM

L. Ortiz*[1]; J. SONG[1]; Y. Zhou[2]; B. Huey[1]

1. University of Connecticut, Materials Science and Engineering, USA
2. Hong Kong Baptist University, Department of Physics, Hong Kong

The performance of thin film solar cells, including chalcogenides as well as halide perovskites, can be strongly dependent on differential properties for grain boundaries and buried interfaces. We have thus employed Tomographic Atomic Force Microscopy (T-AFM) in which nanoscale properties are progressively measured into the depth of the specimen by leveraging sequential material removal via tip-induced surface milling. When configured for photo-conductive AFM, this enables the 3D reconstruction of the network of photoconduction channels within the thin film solar cells. We especially consider partial perovskite solar cell stacks, engineered with distinct back electrodes of SnO_2 or NiO for preferential electron or hole conduction. In this manner, local, ensemble, and depth dependencies of photocurrents can be uniquely assessed to inform improved future solar cell performance.

11:00 AM

(EMA-120-2022) Revealing the Origin of Charge Modulation of 2DEG at $LaAlO_3/SrTiO_3$ Interface by In-situ TEM Biasing (Invited)

S. Oh*[1]

1. Sungkyunkwan University, Energy Science, Republic of Korea

Since its discovery the two-dimensional electron gas (2DEG) forming at $LaAlO_3/SrTiO_3$ (LAO/STO) interface has attracted a lot of research interests of oxide community. Many groups have already demonstrated successful incorporation of 2DEG into field effect transistors or diodes where the field-induced charge modulation is central to the device operation. Although the device technology has been advanced rapidly, the fundamental understanding of the field induced charge modulation is not fully understood. Here we show comprehensive in-situ analysis of LAO/STO system under electrical stimulus in TEM. Our in-situ inline electron holography successfully visualized the field-induced charge density modulation of 2DEG by the electric field applied normal to the LAO/STO interface. While in-situ electron energy loss spectroscopy (EELS) confirmed no measureable oxygen vacancy migration, atom-resolved STEM-HAADF imaging revealed the polar distortion of B-site atoms in both LAO and STO, which induces the ionic polarization gradient across the interface in the range of -18.6 $\mu C/cm^2$ to 18.7 $\mu C/cm^2$ depending on applied voltages. The field-induced polar distortion adds additional charges at the interface with amount depending on the difference between LAO and STO.

11:30 AM

(EMA-121-2022) Atomistic study of site-selective doping behavior in SnO_2

Y. Jin*[1]; W. Jang[2]; Y. Kim[2]; J. Lee[1]

1. Pusan National University, Department of Physics, Republic of Korea
2. SungKyunKwan University, Department of Energy science, Republic of Korea

SnO_2 has been identified as one of the promising and suitable oxide-based photocatalytic semiconductors. However, wide band gap of SnO_2 with rutile crystal structure limits its photocatalytic activity to the visible region. Doping is one of the efficient ways to optimize the materials properties and further enhance the photocatalytic performance. Here, using the first-principles density functional theory calculations, we find that Fe atoms tend to occupy interstitial sites while Cr atoms prefer to occupy substitutional sites accompanied with oxygen vacancies. In particular, substitutional Cr-vacancy cooperation and interstitial Fe-strain coupling produce defect levels in the band gap and introduce excess electrons, narrowing the band gap and sifting the Fermi level up, which significantly improve their photocatalytic properties compared to that of the pristine one. Bandgap narrowing, O-K edge X-ray absorption near edge structure (XANES) spectra due to the oxygen vacancy, and resulting enhanced photocatalytic behavior of visible light will be discussed and associated underlying mechanism will be introduced along with atomic-scale STEM imaging on defective SnO_2.

Wide Bandgap and Ultra-wide Bandgap Semiconductor Thin Films and Heterojunctions

Room: Citrus B
Session Chairs: Bharat Jalan, University of Minnesota; Sriram Krishnamoorthy

2:00 PM

(EMA-173-2022) Theoretical characterization and computational discovery of ultra-wide-band-gap semiconductors (Invited)

E. Kioupakis*[1]

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

Ultra-wide-band-gap (UWBG) semiconductors, i.e., materials with band gaps wider than GaN (3.5 eV) are promising for novel applications in high-power electronics and deep ultraviolet light emitters for water purification and sterilization. Yet, despite decades of research, only a handful of UWBG semiconductors have been developed to date, and they all face challenges with regards to their doping and conduction of electrons and heat. The aim of our work is to apply predictive quantum-mechanical calculations in order to understand the fundamental limitations of current UWBG semiconductors such as Ga_2O_3 and AlGaN, and to discover new materials with improved functionality compared to the current state of the art. Our calculations uncovered the rutile polytype of GeO_2 as a promising UWBG semiconductor with shallow donors and relatively shallow acceptors, high carrier

mobilities, and high thermal conductivity that can overcome the limitations of Ga_2O_3 in power electronics. Moreover, we have discovered several compounds with gaps wider than AlN (6.2 eV) that host shallow dopants and mobile carriers. Our analysis reveals that there is no intrinsic upper band-gap limit that separates semiconductors from insulators and uncovers the rules to design new UWBG semiconductors with improved functional properties.

2:30 PM

(EMA-174-2022) Radiation Damage Effects in Ga_2O_3 Materials and Devices

F. Ren[2]; J. Kim[3]; A. Y. Polyakov[4]; S. Modak[5]; L. Chernyak[5]; A. Haque[6]; S. Pearton*[1]

1. University of Florida, Materials Science and Engineering, USA
2. University of Florida, Chemical Engineering, USA
3. Korea University, Chemical Engineering, Republic of Korea
4. National University of Science and Technology MISiS, Russian Federation
5. University of Central Florida, Physics, USA
6. Pennsylvania State University, Mechanical Engineering, USA

β-Ga2O3 is an ultra-wide bandgap semiconductor attracting interest for power electronics and solar-blind ultraviolet detection. Initial studies of proton, electron, neutron, gamma ray and alpha particle damage have been reported for Ga2O3. In displacement damage measurements, the carrier removal rates are highest for alpha particles and the lowest for gamma rays. Deep electron and hole traps are created, leading to reductions in minority carrier diffusion length and lifetime. Compensation of shallow donors by gallium vacancies interacting with hydrogen is one of the main carrier loss mechanisms resulting from proton damage. Using rectifiers as a platform for studying radiation effects in β-Ga2O3 under conditions relevant to low earth orbit of satellites shows the carrier removal rates for proton, electron and neutron irradiation are comparable to those in GaN of similar doping levels. The main defect created in Ga2O3 by proton irradiation is a relaxed VGa-2H center (Ga vacancy with two hydrogens attached). Electron Paramagnetic Resonance (EPR) after irradiation also shows one dominant paramagnetic defect, which has the characteristics of a VGa -related center. There have been few studies of total ionization dose or single event upsets in Ga2O3 and while the former is not expected to be significant because of the lack of gate oxides in most device structures in this materials system, single event upsets may be an issue.

2:45 PM

(EMA-175-2022) Nitrogen Ion-Implanted Resistive Regions for Edge Termination of Vertical Ga_2O_3 Rectifiers

X. Xia*[1]; M. Xian[1]; C. Fares[1]; R. Sharma[2]; M. Law[2]; F. Ren[1]; S. Pearton[2]

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

Design and implementation of N implanted edge termination in vertical geometry Ga_2O_3 rectifiers were investigated. Ultra-wide bandgap semiconductor β-Ga_2O_3 has attracted increasing attention because of the prospects for use in high-performance power switching electronics. In the case of high-voltage devices, edge termination plays an extremely crucial role in determining the breakdown voltage. N^+ ion implantation to form resistive regions for edge termination at the anode contact periphery was used to maximize the breakdown voltage (V_B) of vertical geometry β-Ga_2O_3 rectifiers. The design was examined via simulations using the FLOODS/ FLOOPS TCAD simulator. The configuration of the implanted region was investigated with these simulations and then implemented experimentally. Significant increases of ~200-250% in V_B were achieved for 50-1000μm diameter rectifiers with an unbounded resistive region and an implantation depth of ~0.5 μm. The on-state resistance and on/off ratios of the rectifiers was essentially unchanged by the addition of the implanted regions. An optimized implanted edge termination structure maximizes breakdown voltage with no associated increase in device resistance in vertical geometry Ga_2O_3 rectifiers.

3:00 PM

(EMA-176-2022) Approaches Towards Oxide-Nitride Heterojunctions (Invited)

V. Wheeler*[1]; D. R. Boris[1]

1. Naval Research Laboratory, USA

Next generation devices will require novel heterojunctions, often between dissimilar materials, to overcome the limitations of a singular system. New approaches are needed to promote epitaxial films with proper structure and properties, as well as abrupt, pristine interfaces necessary for device applications. We will examine a few oxide/nitride heterojunction examples to discuss the critical aspects and possible solutions for advancing heterogeneous heterojunctions. First, we demonstrate a low temperature fluorine-based plasma process to simultaneously remove the AlN native oxide and passivate the surface with a stable fluorine film. This allows for abrupt, pristine, epitaxial heterojunctions using a process that is typically inhibited by the inability to remove deleterious interfacial oxides. We also show the direct integration of metastable, polar ε Ga2O3 with GaN using a plasma-enhanced ALD process. ε Ga2O3 theoretically has a higher polarization than III-N's, leading to 2DEG channels with higher charge and mobility for devices. Lastly, integrating functional epitaxial oxides can improve device performance. $Sr_{1-x}Ca_xTiO_3$, with both a high dielectric constant and antiferroelectric/ferroelectric states, was integrated on GaN and AlGaN using a thin TiO_2 buffer layer to overcome lattice and structural mismatches. For all cases, we will present structural, chemical and morphological data resulting from these unique heterojunctions.

4:00 PM

(EMA-177-2022) Shining the Spotlight on Defects in β-Ga_2O_3 (Invited)

M. Scarpulla*[1]

1. University of Utah, USA

The properties of Ga_2O_3 places it squarely at the interface between the fields of semiconductor and ceramics science and engineering. In polycrystalline form, it has seen wide use in gas sensing applications, while recently the availability of large melt-grown β-Ga_2O_3 single crystals has enabled investigations of its use in semiconductor power devices and UV detectors. The primary differentiating property for β-Ga_2O_3 is its high breakdown field, however the roles of defects in determining other properties such that this intrinsic property can be harnessed must be illuminated – figuratively shining a spotlight on β-Ga_2O_3 defects. Defect physics and engineering are at the heart of understanding and optimizing the material for these applications. I will detail efforts to understand impurities and native defects in both bulk melt grown crystals and epitaxial films. First, changes in native defects upon annealing in oxygen will be discussed. This connects also to diffusion of vacancies and impurities from bulk-grown crystals into epitaxial films and allows determination of the cation vacancy self-diffusion coefficient. Changes in defect populations are discovered upon bias and temperature stressing of devices. Finally, illumination – literally shining a spotlight on β-Ga_2O_3 - is shown to be capable of modifying the types and concentrations of defects, opening up whole new avenues of processing to achieve desired sets of properties.

4:30 PM

(EMA-178-2022) Atomic-scale Characterization of Non-uniform γ-Ga_2O_3 Phases in Sn ion-implanted β-Ga_2O_3 Films

T. J. Yoo*[1]; X. Xia[2]; F. Ren[2]; M. Tadjer[3]; S. Pearton[1]; H. Kim[1]

1. University of Florida, Materials Science and Engineering, USA
2. University of Florida, Chemical Engineering, USA
3. U.S. Naval Research Laboratory, USA

β-Ga_2O_3 (monoclinic) continually garners interest as an ultra-wide bandgap (UWBG) semiconductor for high power electronics applications owing to its bandgap of ~4.8 eV and high electric breakdown field of 8 MV cm^{-1}. Doping by ion implantation has been studied extensively for other material systems (e.g. Si, SiC, and GaN). However, there is a lack of knowledge on the structural effects of ion implantation on β-Ga_2O_3 along with the resulting impact on electrical properties. We characterized the atomic-scale structure of Sn ion-implanted β-Ga_2O_3 thin films using aberration-corrected scanning transmission electron microscopy as well as energy dispersive x-ray spectroscopy to reveal the chemical distribution across the doped region. We report the presence of a non-uniform defect phase near the surface of the implanted film, identified as different orientations of the γ-Ga_2O_3 (cubic) phase formed during the highly energetic doping process. This talk will include discussion on the potential consequences of such defect phases as well as future directions for the investigation of ion implanted β-Ga_2O_3 to achieve better optimized doping procedures.

4:45 PM

(EMA-179-2022) Growth and Interface Characterization of In-situ MOCVD-grown Al_2O_3 Dielectric/(010) β-Ga_2O_3 Interface

S. Roy*[1]; A. Chmielewski[2]; A. Bhattacharyya[3]; P. Ranga[3]; R. Sun[3]; M. Scarpulla[3]; N. Alem[2]; S. Krishnamoorthy[1]

1. University of California, Santa Barbara, Materials, USA
2. Pennsylvania State University, Department of Material Science and Engineering, USA
3. University of Utah, Department of Electrical and Computer Engineering, USA

We report on the growth and characterization of in-situ Al_2O_3 on (010) β-Ga_2O_3 using metalorganic chemical vapor deposition (MOCVD) as a better alternative to the most commonly used atomic layer deposition (ALD) technique. To extract trap densities and electrical properties of the in-situ Al_2O_3/ β-Ga_2O_3 interface, three metal oxide semiconductor capacitor (MOSCAP) structures with three different Al_2O_3 thicknesses were fabricated. The growth of Al_2O_3 is performed in the same reactor as β-Ga_2O_3 using Trimethylaluminum and O_2 as precursors without breaking the vacuum at a growth temperature of 600 °C. A stable positive fixed charge of +2 x 10^{12} cm^{-2} is calculated from the CV hysterisis plot. The sheet density of near interface trap states with fast and slow emission times were found to be 1.2 x 10^{12} cm^{-2} and 3 x 10^{11} cm^{-2} respectively. The density of all the interface states (D_{it}) and their energy dependences were characterized using deep ultra-violet (DUV) assisted CV technique. An average D_{it} of ~6.4 x 10^{11} cm^{-2} eV^{-1} is calculated, which is significantly lower than the ALD Al_2O_3/ β-Ga_2O_3 interface from literature. Band offset of the in-situ Al_2O_3/ β-Ga_2O_3 heterostructure is also calculated to be 1.7 eV. An average peak breakdown field of approximately 5.6 to 5.8 MV/cm underneath the center of the anode is extracted using forward and reverse IV characteristics.

5:00 PM

(EMA-180-2022) Self-assembled superlattice structures on nominal InGaN films grown by plasma-assisted molecular beam epitaxy (Invited)

E. Ahmadi*[1]

1. University of Michigan, USA

The InGaN alloy system is attractive for a variety of optoelectronic applications, including laser diodes (LDs), light-emitting diodes (LEDs), and photo-detectors, as it enables direct bandgap tuning within a large range (0.7 eV–3.4 eV). The (In,Ga)N material system is also attractive for photovoltaic applications as its optical absorption covers the solar spectrum. In this talk, I will give an overview of our recent progress on high-temperature growth of InGaN films by plasma assisted molecular beam epitaxy (PAMBE) on different substrates including ZnO, Ga-polar GaN, and N-polar GaN. I will present observation of spontaneous formation of $In_{0.2}Ga_{0.8}N$/GaN and $In_{0.26}Ga_{0.74}N$/GaN superlattice structures with excellent structural quality on nominal InGaN films grown on Ga-polar and N-polar GaN, respectively, by PAMBE. We studied the impact of strain on the superlattice formation by growing InGaN on ZnO using similar growth conditions. The self-assembled superlattice grown on ZnO showed less modulation in the In incorporation. Additionally, InGaN films grown at lower temperatures (e.g. 560 °C) did not show any superlattice structure. These observations suggest that the self-assembled superlattice structure may be due to vertical phase separation of InGaN caused by high temperature growth and intensified by strain.

5:30 PM

(EMA-181-2022) Identification of Point Defects and Alloy Distribution in β-$(Al_xGa_{1-x})_2O_3$ Heteroepitaxy

H. Huang*[1]; J. M. Johnson[1]; C. Chae[1]; M. Wang[3]; S. Mu[3]; A. Bhuiyan[2]; Z. Feng[2]; N. K. Kalarickal[2]; S. Rajan[2]; H. Zhao[2]; C. Van de Walle[3]; J. Hwang[1]

1. Ohio State University, MATERIALS SCIENCE AND ENGINEEING, USA
2. Ohio State University, Electrical and Computer Engineering, USA
3. University of California, Santa Barbara, Materials Department, USA

Gallium oxide has emerged as one of the promising candidates for ultra-wide bandgap materials for future power electronics applications. To further enhance channel mobility and achieve tunable bandgap, $(Al_xGa_{1-x})_2O_3$ has been under development by alloying Al into Ga_2O_3. For this effort, a clear understanding of the formation of point defects and their complexes, as well as the alloy incorporation at the atomic scale is critically required. We aim to provide such detailed information from β-$(Al_xGa_{1-x})_2O_3$ thin films using quantitative scanning transmission electron microscopy (STEM). Our quantitative analysis of atomic column intensities in STEM images reveals the details of atomic arrangement and point defects. For $(Al_xGa_{1-x})_2O_3$ films with varying x, we show that the Al atoms occupy on both octahedral and tetrahedrally coordinated sites with an estimated ratio of (54:46), which is in contrast to bulk film and highlights the surface diffusion kinetics involved in non-equilibrium conditions in epitaxy. Furthermore, our analysis revealed that the planar defects observed in these films resemble the structure of r-phase Al_2O_3, which can impede the heteroepitaxy beyond a certain critical film thickness. In summary, quantitative STEM analysis provides atomic scale features of defect formation and alloy distribution in $(Al_xGa_{1-x})_2O_3$ films, which help understand the growth mechanism and properties.

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

2D Materials and Low Dimensional Conductors I

Room: Orange B
Session Chair: Bing Lv, University of Texas, Dallas

10:00 AM

(EMA-122-2022) Efficient Control of 2D Magnetism (Invited)

C. Gong*[1]

1. University of Maryland, USA

Emergent two-dimensional (2D) magnetic materials hold great promise for efficient control of magnetism, fundamentally owing to their 2D nature. However, thus far, there have been only proof-of-concept reports on electrical and optical control of 2D magnetism. There appear to be some fundamental obstacles for the efficient control. In this talk, I will analyze the challenges and present our recent theoretical and experimental progress on efficient electrical and optical control of 2D magnetism. Specifically, our results show that the continuous wave laser of 10s of uW/um^2 can effectively change the domain behaviors in 2D magnets, and 100 mV/nm electric field can effectively change the magnetic anisotropy of 2D magnets. We envision the efficient control of 2D magnets could open new avenues to the miniaturized low-power spintronics.

10:30 AM

(EMA-123-2022) Synthesis, formation mechanism and electronic properties of one-dimensional van der Waals heterostructures (Invited)

R. Xiang*[1]; S. Maruyama[1]

1. The University of Tokyo, Japan

We present the experimental synthesis of one-dimensional (1D) van der Waals heterostructures, a class of materials where different atomic layers are coaxially stacked. A typical structure is a 5-nanometer–diameter heteronanotube consisting of an inner SWCNT, a middle three-layer BN nanotube (BNNT), and an outer MoS_2 nanotube (MoS_2NT). Electron diffraction verifies that all shells in this structure are single crystals. This work suggests that all of the materials in the current 2D library could be rolled into their 1D counterparts and a plethora of function-designable 1D heterostructures may be realized. We also present our recent follow-up study on the structural details and formation mechanism of 1D heterostructures. Edge structures, nucleation sites, crystal epitaxial relationships are clearly revealed using a nondestructive transmission electron microscopy. Finally, we present the initial results on the electronic transport of 1D heterostructures, including a radial semiconductor–insulator–semiconductor heterojunction using a SWCNT-BNNT-MoS_2NT. We expect that 1D heteronanotubes can serve as new building blocks for various electronic and optical devices.

11:00 AM

(EMA-124-2022) Emergent transport properties in superconducting tungsten disulfide nanotubes (Invited)

T. Ideue*[1]

1. The University of Tokyo, Japan

Nanotube has a unique geometrical structure, symmetry, and dimensionality, which strongly affect the electronic states and physical properties. Especially, novel superconducting transport are expected in superconducting nanotubes. Although superconductivity in the assembled form of single, double or multi-walled nanotubes have been already reported, relations between superconducting properties and characteristics of the nanotube are still unclear. Here we report a new superconducting nanotube of inorganic tungsten disulfide realized by the electrolyte gating technique and exotic quantum transport originating from the nanotube structures. Quantum interference reflecting the cylindrical structure (Little-Parks effect) has been observed, from which we can estimate the effective diameter of the superconducting nanotubes. We also found the systematic variation of the superconducting transition temperature as a function of the effective diameter of the nanotube. Moreover, effect of chirality on the superconducting transport has been probed for the first time as the magnetochiral anisotropy (intrinsic rectification effect originating from the symmetry breaking), which is significantly enhanced in the superconducting state and associated with Little-Parks oscillations. Our results offer a new material platform of low dimensional superconductivity and unique characteristics /functionalities in nanotubes.

11:30 AM

(EMA-125-2022) Magnetism and Superconductivity in 2D Layered metal Thiophosphates (Invited)

M. A. Susner*[1]; B. S. Conner[1]; B. Lv[2]; R. Rao[1]

1. The Air Force Research Laboratory, USA
2. University of Texas, Dallas, USA

Correlated two-dimensional (2D) materials offer a new avenue for the development of next-generation electronic devices. Since the discovery of Dirac physics in graphene, research in 2D materials has grown exponentially with two main aims: 1) the discovery of new 2D materials and 2) developing new and innovative techniques to harness and tune their optical, magnetic, and electronic properties. Though most research on 2D materials has focused on graphene, boron nitride, and transition metal chalcogenides (TMCs), new 2D materials classes are coming into the forefront, including metal thiophosphates which, in many ways, are the 2D equivalent of complex oxides as changes in composition, stacking, or pressure in turn lead to large changes in bandgap, magnetic ordering temperature and type, ferroelectric ordering temperature, possible Kitaev physics (i.e. quantum spin liquids) and even the appearance of superconductivity. In this talk I shall review the proprties known in the literature for this family and the interplay between chemistry, structure, magnetism, and superconductivity followed by a discussion of our work thus far and possible routes for future investigation.

12:00 PM

(EMA-126-2022) Superconducting nanowire yarn consisting of NbN on dry-spun carbon nanotube sheets followed by the twist insertion (Invited)

D. Suh*[1]

1. SungKyunKwan University, Department of Energy Science, Republic of Korea

We have fabricated a superconducting nanowire yarn consisting of carbon-nanotube (CNT) templated sputter-deposited NbN nanofibrils. The superconducting properties of NbN is maintained in the highly porous yarn structure, where a thin layer of NbN is surrounding individual CNT nanofibrils and bundles. Proper engineering to lower the normal state resistance could be applied by the additional deposition of other metallic materials. From a careful analysis, furthermore, we found out that an anomalous absolute negative resistance could appear instantaneously during the superconducting transition process in some cases due to the distortion of charge conduction paths. Concerning its mechanical properties, the superconductivity of this NbN nanowire yarn is maintained even under the condition of large deformation, but its superconducting properties in its pristine state are degraded. To solve this issue, we develop an annealing method of Joule heating up to the stage of incandescent light emission, which greatly enhances the superconducting properties of the NbN nanowire to reach the literature record level. Such a property improvement can be understood from the morphology change of the internal structure of the yarn.

2D Materials and Low Dimensional Conductors II

Room: Orange B
Session Chair: John Bulmer, Air Force Research Lab (AFRL)

2:00 PM

(EMA-182-2022) Electronic transport in ultrahigh-conductivity aligned carbon nanotube assemblies (Invited)

N. Komatsu*[1]

1. Rice University, Electrical and Computer Engineering, USA

Macroscopic assemblies of aligned carbon nanotubes (CNTs) with ultrahigh conductivity (> 10 MS/m) have recently become available. They are promising for diverse applications, including power transmission and thermoelectric energy harvesting, but the transport mechanisms are not well understood. In particular, the roles of disorder, doping, and electron-electron interactions have not been elucidated. Here, we describe our recent temperature- and magnetic field-dependent conductivity measurements on aligned CNT fibers, bundles, and films, produced by the solution spinning method. Fiber samples exhibited positive temperature coefficients of resistance in a wide temperature range (30-300 K), distinctly different from many previous reports. At low temperatures, we observed strongly temperature-dependent negative magnetoresistance, a hallmark of weak localization, suggesting quantum coherent transport. To determine the dimensionality and coherence lengths of carriers from the weak localization behavior, we conducted magnetic field-dependent conductivity measurements on individual crystalline CNT bundles. Finally, we performed Hall measurements on films to compare with previous studies performed in strongly localized regimes. These extensive and systematic transport studies on aligned CNT assemblies provide insight into the transport mechanisms and strategies for further conductivity improvement.

2:30 PM

(EMA-183-2022) Magnetoresistance of chemical vapour deposition spun carbon nanotube fibers (Invited)

A. Lekawa-Raus*[1]

1. Warsaw University of Technology, Poland

Synthesis of carbon nanotube (CNT) fibers via floating catalyst chemical vapour deposition method (FC-CVD) provides a unique opportunity of altering morphology of CNT fibers via a change of feedstock and process conditions. Here we present the results of magnetoresistance (MR) measurements performed for 3 types of samples: a) very clean fibers comprising only armchair single wall nanotubes synthesized using carbon disulphide as a sulphur precursor and methane as a hydrocarbon, b) very densely packed fibers produced using thiophene and ethanol which comprised mainly long (up to 1mm) single, double and triple wall nanotubes of various chiralities, c) the poorest quality CNT fibers produced using thiophene and hexane. Some of the methane fibers were additionally doped via immersion in nitric acid. The magnetoresistance tests conducted at temperatures from 1.17 K up to 230 K and up to 60T showed clear differences in the performance of the samples. All samples showed an initial negative MR which next turned to positive MR with a point of change dependent on temperature and type of sample. The positive MR effect was also observed to decrease with better quality and doping of the samples. For the doped samples the threshold of positive MR was clearly beyond 60 T in the temperature range from 30-90 K. The following talk will discuss the MR behavior and transport models in relation to the fibers morphology.

3:00 PM

(EMA-184-2022) Semiconducting Single-Walled Carbon Nanotube Yarns Fabricated via Wet-Spinning (Invited)

W. Yu*[1]; Y. Kim[1]; H. Yang[1]; Y. Kim[1]; J. Lee[1]

1. Seoul National University, Material Science and Engineering, Republic of Korea

We fabricated semiconducting single-walled carbon nanotube (sc-SWNT) fibers via wet-spinning for biosensor platforms and thermoelectric devices. SWNTs were purified using thermal and acid treatments and separated into metallic SWNTs and sc-SWNTs. The sc-SWNTs were then wet-spun into flexible fibers. To investigate the potentials of sc-SWNT yarn to biosensor platform application, an enzyme capable of reacting with glucose was immobilized on the sc-SWNT fibers. The enzyme-activated sc-SWNT fibers, which exhibited the field effects, were then configured into fiber-type glucose sensors capable of detecting the glucose in a solution, demonstrating the potential of sc-SWNT fibers as an electrochemical biosensor platform. On the other hand, we developed a novel processing method (electric potential-applied wet spinning) to increase the strength of fibers and thus use sc-SWCNT fibers in wearable devices. The mechanical strength of SWCNT fibers was increased by about 181% due to the alignment of SWNTs caused by the electrical potential. Finally, sc-SWCNT fibers were doped using p-type and n-type dopants, respectively, and the effect of doping was confirmed by measuring the seebeck coefficient. We are carrying out a series of research to develop all carbon thermoelectric 3D textiles, the results of which will be presented at the conference.

4:00 PM

(EMA-185-2022) Electrical and mechanical properties of high electrical conductivity CNT/Cu-yarns with Br doping and various encapsulations (Invited)

M. D. Sumption*[1]; S. xue[1]

1. Ohio State University, MSE, USA

In this work, we pursued the development of high specific electrical conductivity and high specific strength CNT/composites. We started with CNT yarns which had an initial electrical conductivity, σe, of 3.14MS/m and a density of 1.32 g/cm. We brominated the yarns, demonstrating increases in σe, with our best samples reaching σe = 7.00 MS/m. To increase the stability of the bromination, we electroplated a Cu layer onto the B-doped yarn which led to a stabilization of the conductivity improvement. This was quantified by monitoring periodically the σe of a Br-doped and metallized CNT yarn over a period of 69 days, during which time the sample was otherwise exposed to ambient conditions. Analysis gives a value 6.15 MS/m for the brominated yarn after metallization which is excellent for CNT yarns. Tensile tests on these Cu/CNT composites showed tensile strengths reaching 700 MPa, Young's modulus values of 22.8 GPa, and specific tensile strength values of 146 kN*m/kg (this latter is 6X that of Cu). Our best CNT-Cu composites show specific conductivity values comparable with that of Cu but with much higher specific tensile strengths. We have also explored CNT yarns encapsulated with conductive polymers. We have attempted brominization on these composites, with pre- and post-encapsulation protocols. Results are discussed and compared to metallic encapsulations.

4:30 PM

(EMA-186-2022) Effects of carbon nanotube length on magneto-transport of de-doped/Li-doped/SbF5-doped solution spun fibers (Invited)

J. Bulmer*[1]

1. Air Force Research Lab (AFRL), USA

Solution spun carbon nanotube (CNT) fibers now are on a level of conductivity, mechanical strength, stability, and availability that surpasses the most practical graphitic intercalation compounds (GIC); the most graphetically pristine (and fragile) GICs however still exceed CNTs in respect to extremes in absolute conductivity (GIC conductivity ~150% Cu, CNT conductivity ~17% Cu). In this talk we will first review CNT and GIC state of the art and discuss contrasting characteristics. Next, we show experimental resistance dependence on temperature (400 to 1.9 K) and magnetic field (0 to 9T) for solution spun CNT fibers with different average CNT lengths. We completely de-dope the solution spun CNT fibers from their residual acid with a 1300 K hydrogen-based annealing without sacrificing graphitic quality. We also re-introduce doping chemical species (lithium and antimony pentafluoride) and observe effects on transport. In the de-doped state, CNT fibers with different length distributions show signatures of variable range hopping (instead of fluctuation induced tunneling) at the coldest temperatures; metallic features start appearing at warmer temperatures and for fibers with longest CNTs. Li-doping greatly reduces the semi-conducting features of the transport. For SbF5-doping to be effective, fibers must first be de-doped to prevent reacting with the residual acid.

5:00 PM

(EMA-187-2022) Low Temperature Properties of Carbon Nanotubes Bundles and Fibers (Invited)

M. Cirillo*[1]

1. Università di Roma "Tor Vergata", Dipartimento di Fisica and MINAS Lab, Italy

Beginning from the Quantum Hall Effect, passing through High Temperature Superconductors, Carbon Allotropes and Organic Perovskites the chemico-physical behavior of low-dimensional structures has gained increasing appeal in condensed matter and material science. Many issues remain open, but it is clear now that the structural anisotropy plays a paramount role in determining their behavior. The peculiar, quasi one-dim structure of carbon nanotubes (CNT) bundles and fibers lends itself to intriguing investigations and speculations in this field. I will review aspects of CNT bundles and fibers that we have been investigating in the past decade focusing the attention on transport properties and possible applications for radiaction detection or as "cores" to be coated in superconducting wires technology. The transport properties of these systems, performed in a temperature interval ranging from 4K up to 300K, are interpreted on the basis of models invoking fluctuation-induced tunnelling and consistency of the applied model is found from measurements performed in dark and under laser illumination. I also review results obtained from doping CNT fibers with potassium or nickel, an investigation that was performed bearing in mind that interesting properties of low-dimensional systems can be displayed when the these are doped with impurities or when charge reservoirs are around in layered structures.

5:30 PM

(EMA-188-2022) Synthesis of MnO_2 Carbon Nanotubes catalyst with enhanced Oxygen Reduction Reaction for Polymer Electrolyte Membrane Fuel Cell (Invited)

A. Ullah*[1]

1. University of science and Technology South Korea, Energy, Republic of Korea

Polymer Electrolyte Membrane Fuel Cell (PEMFC) is an electrochemical cell which undergoes oxygen reduction reaction to produce energy. Platinum (Pt) metal has been used for catalysis since its inception but expensiveness is the major obstacle in commercialization of fuel cell. Herein a non-precious group metal (NPGM) is employed instead of Pt to reduce the cost of PEMFCs. Manganese dioxide based carbon nanotubes (MnO_2 CNTs) is a catalyst having excellent electrochemical properties and offers a better alternative to the Platinum based PEMFC. To enhance the catalytic activity and increase the volumetric current density, the sample was pyrolyzed at 800 °C temperature under nitrogen atmosphere. The catalyst has been characterized by scanning electron microscope (SEM), X-ray diffraction (XRD) and the catalyst activity has been examined by Rotating Disc Electrode (RDE) experiment. Linear Sweep Voltammetry (LSV) depicts a excellent current density of -4.0 mA/cm^2 and an over potential of -0.3V vs. Standard Calomel Electrode (SCE) in 0.1M KOH electrolyte. Rotating Disk Electrode (RDE) was conducted at 400, 800, 1200, and 1600 rpm. The catalyst exhibited a higher methanol tolerance and long term durability with respect to commercial Pt/C. The results of MnO_2CNT show that the low cost catalyst will supplant the expensive Pt/C catalyst in the fuel cell.

S10: Point Defects and Transport in Ceramics

Defect Mobility and Transport Behavior

Room: Cypress B

Session Chair: Kaveh Ahadi, NCSU

10:00 AM

(EMA-127-2022) Electromigration of Oxygen Vacancies and Better Prediction of Failure of Multilayer Ceramic Capacitors (Invited)

C. Randall*[1]; P. Yousefian[2]

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

Multilayer ceramic capacitors (MLCCs) are a critical part of all electrical systems. With new applicationareas in electrification of automobiles, 5G, computation, energy control, etc., the number of capacitors is increasing at arapid rate. With capacitors functioning with high voltages across the dielectric layers, this means that minority chargecarriers can drive a failure of the components. This means the weakest electric components in all these electrical circuitsand systems is often linked to the individual failure of these capacitor components. So, with the large numbers ofcapacitors and the more hostile electrical and temperature operational conditions, we must pay more attention to thedefect migrations in such components. In this talk, we will review the point defect failure mechanisms and providedetailed considerations on the local damage that can occur in a burn-in test that is used to screen out weak componentsfor high reliability applications for MLCCs. The technique of thermally stimulated depolarization current is a verypowerful method to understand the electromigration of oxygen vacancies and will be used to assess burn-in damage. Thisprovides a powerful insight into the intergranular and transgranular electromigration of the dielectric ceramics.

10:30 AM

(EMA-128-2022) Determining the Effect of Burn-in Process on Dynamics of Oxygen Vacancies in X7R Multilayer Ceramic Capacitors

P. Yousefian*[1]; C. Randall[1]

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

Base metal electrode (BME) multilayer ceramic capacitors (MLCC) are being considered in aerospace, medical, and military applications and thereby need to hold higher levels of reliability. Thus, it is essential to determine the reliability of MLCC components in terms of their lifetime. Burn-in or screening process has been used to remove components with higher probabilities of infant mortality failures. In this process, components are exposed to both high temperatures and high voltages for a certain period of time. Migration of oxygen vacancies is the most acknowledged degradation mechanism of MLCCs under the dc bias. In this study, electrical characterization techniques like Thermally Stimulated Depolarization Current (TSDC) and Highly Accelerated Lifetime Testing (HALT) were used to study the time dependences phenomena occurring over the burn-in conditions with special consideration to electromigration of oxygen vacancies space charge distributions. Experimental results demonstrated that the aggressive burn-in process can lead to intragranular and transgranular oxygen vacancies electromigration, which can reduce the lifetime of MLCC components by compromising the double Schottky barriers at the grain boundaries and electrode interfaces.

10:45 AM

(EMA-129-2022) The role of defects on the ionic conductivity in yttria-stabilized zirconia (Invited)

B. Feng*[1]; N. Shibata[1]; Y. Ikuhara[2]

1. The University of Tokyo, Japan
2. University of Tokyo, Institute of Engineering Innovation, Japan

Yttria-stabilized zirconia (YSZ) is one of the primary choices for the electrolyte material in fuel cell technologies due to its excellent ionic conductivity. However, the performance is known to be largely affected by the lattice defects inside, e.g. grain boundaries (GBs) and dislocations. In this study, we have investigated the role of these defects using atomic-resolution scanning transmission electron microscopy (STEM). Well-oriented model GBs and dislocation arrays were fabricated by bicrystal method using thermal diffusion bonding of two 10YSZ single crystals at 1600 °C for 15 hours. Atomic-resolution STEM observation was performed for structural characterization. For the YSZ GBs, STEM-EDS results show that Y atoms tend to segregate at the GB, and the relative oxygen concentration in the GB is increased compared with the bulk. Therefore, the oxygen vacancies are depleted in GBs, which could lead to a high resistivity at the GB. For the YSZ dislocation, we first quantified the fractional change of the volume and Y segregation around the dislcocation core. Based on the previously reported strain-conductivity and chemistry-conductivity relationships in YSZ, we mapped out relative ionic conductivity change at the dislocation. We found that the a faster ionic condcutivity path can be formed due to the coupling of the tensile strain field and Y segregation.

11:15 AM

(EMA-130-2022) Low temperature cation and anion diffusion in single crystal Fe_2O_3

T. Kaspar*[1]; K. Yano[3]; A. A. Kohnert[2]; B. Matthews[3]; S. R. Spurgeon[4]; Z. Zhu[5]; D. Schreiber[3]

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
2. Los Alamos National Lab, Materials Science and Technology, USA
3. Energy and Environment Directorate, Pacific Northwest National Laboratory, USA
4. Pacific Northwest National Laboratory, Energy and Environment Directorate, USA
5. Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, USA

The diffusion of cations and anions in the ubiquitous corrosion product hematite, α-Fe_2O_3, has been of interest for several decades. Historically, studies of Fe and O diffusion through the oxide lattice have been limited to temperatures greater than approximately 900°C to achieve measurable diffusion in a reasonable timeframe. Recently, our group has predicted a changeover in anion transport to an interstitialcy mechanism at temperatures below 850 – 1000°C. Here, we present results from high-precision, nanoscale cation and anion diffusion experiments using isotopically labeled α-Fe_2O_3 at 650°C to evaluate transport mechanisms at a much lower temperature. Epitaxial α-Fe_2O_3 films were deposited on single crystal Al_2O_3(0001) (c-plane) and Al_2O_3(11-20) (a-plane) substrates by oxygen-plasma-assisted molecular beam epitaxy, with a 10 nm thick ^{57}Fe and ^{18}O enriched tracer layer of Fe_2O_3 placed within each thin film. Isotopic tracer distributions were measured after thermal annealing with secondary ion mass spectrometry and atom probe tomography. Extracted cation and anion diffusion rates are compared to model predictions to elucidate transport mechanisms, and the impact of these mechanisms on radiation-enhanced diffusion will be discussed.

11:30 AM

(EMA-131-2022) Oxygen vacancy and polarization dynamics in $(Bi_{0.5}Na_{0.5})TiO_3$ ferroelectrics

Z. Fan*[1]; C. Randall[2]

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

BNT is currently a very hot topic among the lead-free piezoceramic community due to its potential usage in actuators or energy storage capacitors. The naturally formed Bi vacancy, in combination with any acceptor/donor dopants, gives rise to very complicated defect kinetics in BNT, which will decisively impact the performance and the reliability. In this presentation, we will cover several aspects, important but poorly comprehended, related to the oxygen vacancy dynamics and the relaxor ferroelectric behaviors, plus some comments on the correlation between these two. For instance, ionic conduction in relaxor and ferroelectric phase; dc degradation; conduction mechanisms in BNT-xBT solid solution; stability of ferroelectric ordering against defects introduction; history dependence of dielectric relaxation, etc.

11:45 AM

(EMA-132-2022) Point defect transport and self-diffusion in hematite and chromia thin films (Invited)

A. A. Kohnert*[2]; A. Banerjee[2]; K. Yano[1]; T. Kaspar[1]; E. F. Holby[3]; D. Schreiber[1]; B. P. Uberuaga[2]

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
2. Los Alamos National Laboratory, Materials Science and Technology Division, USA
3. Los Alamos National Lab, Sigma Division, USA

Formation and transport of point defects in oxides is key to the growth, stability, and protectiveness of passivating layers on metals. Advances in both theoretical methods and experimental techniques capable of accessing the atomic scale can investigate transport in conditions unavailable to bulk techniques, and provide fundamental information on point defect properties and behavior. This study applies a multi-scale model to investigate mass transport through corundum structured oxide films beginning with density functional theory calculations of point defect formation and migration energies. These properties are coupled to a reaction-diffusion framework to predict the evolution of point defect concentrations and fluxes in response to changing temperature, chemical environment, or radiation exposure. Finally, these predictions are compared to the observed mass transport and self-diffusion extracted from atom probe tomography measurements of isotope tracer redistribution.

S14: Functional Materials for Biological Applications

Functional Materials for Biological Applications

Room: Cypress B

Session Chairs: Jennifer Andrew, University of Florida; Julia Glaum, NTNU

2:00 PM

(EMA-189-2022) Active microenvironments for tissue regeneration and related applications (Invited)

S. Lanceros-Mendez*[1]

1. BCMaterials, Basque Center for Materials, Applications and Nanostructures, Spain

Active, smart and multifunctional materials are increasingly needed in tissue regeneration and biomedical applications in order to provide specific clues to the cells. In particular, the use of electroactive polymers that deliver electrical signals to the cells upon mechanical, magnetic or thermal solicitation, open new scientific and technological opportunities, allowing the development of specific biomimetic microenvironments for tissue regeneration. In fact, electrical and electromechanical clues are among the most relevant ones in determining tissue functionality in tissues such as muscle and bone, among others, indicating their requirement for proper tissue regeneration. This talk reports on smart and multifunctional active materials, such as piezoelectric and magnetoelectric, tailored for tissue engineering applications in terms of size, shape and functionality. The most used materials and morphologies are reported, together with specific bioreactor designs allowing to take full advantage of those materials. The main achievements, challenges and future needs will be presented and discussed. Acknowledgements Spanish State Research Agency (AEI): PID2019-106099RB-C43 / AEI / 10.13039/501100011033. Basque Government Industry and Education Department: ELKARTEK and PIBA programs.

2:30 PM

(EMA-190-2022) Functional Materials: Definition, Origin and Improvement of Functionality of Materials (Invited)

M. Yoshimura*[1]

1. National Cheng Kung University, Mater. Sci. & Eng., Taiwan

In general, materials would be defined as [I] Functional materials and [II] Structural materials. However, it has not been clear "What is the definition and Origin of functionalities in materials." Functional materials mean that materials act for transfer, move change, react with external fields and/or environments, that is, functional materials are active and/or reactive for out-side signal, fields and/or species. In this regard, functional materials should involve weakly bonded parts in their compositions and/or structures. If this definition could be accepted, improvements of functionalities require the increase and/or enhancement of active parts (= weakly bonded parts) by doping, modification, defects and/or surface and interface. On the other hand, properties like Optical transparency (no absorption), Insulation (no conduction), Thermal conduction (no absorption and scattering), which would be regarded as Functions, might not be "Function", but rather "Anti-Function", like Stiffness, Break-down, Fracture strength, Melting, Anti-corrosion, Anti-oxidation, etc. They would prefer Inactive thus hate weakly bonded parts (= active and reactive parts). Thus, improvement of "Anti-Function" should be opposite direction of the improvement of "Function".

3:00 PM

(EMA-191-2022) Piezoelectric components for active hearing implants (Invited)

T. M. Eßinger[1]; M. Koch[1]; M. Bornitz*[1]; M. Neudert[1]

1. Technische Universität Dresden, Faculty of Medicine Carl Gustav Carus, Germany

Hearing loss with a sensorineural component often calls for active implants that provide electric or acoustic stimulus. There's a large variety of such implants, but all have one thing in common: The need for acoustic sensors. The current demand for the development of fully implantable devices means that such sensors must be small, durable, and easy to handle, while at the same time providing high sensitivity and dynamic range. Piezoelectric components are promising candidates both as implantable sensors and actuators. We provide an overview of the most notable current research in this area, with a focus on our own development of an implantable sensor/actuator inside the ossicular chain. The design is built around single crystal PMN-PT elements that act as a force sensor or sensor/actuator. Laboratory studies in human temporal bone specimens show the potential of the design in the context of both cochlear implants and active middle ear implants. Compared to state-of-the-art implantable microphones, it offers advantages in handling, surgery, and bodynoise decoupling.

3:30 PM

(EMA-192-2022) Ultra-compact Dual-band Smart NEMS Magnetoelectric Antennas for Simultaneous Wireless Energy Harvesting and Magnetic Field Sensing (Invited)

M. Zaeimbashi[1]; M. Nasrollahpour[1]; A. Khalifa[2]; A. Romano[1]; X. Liang[1]; H. Chen[1]; N. Sun[1]; A. Matyushov[1]; H. Lin[1]; C. Dong[1]; Z. Xu[1]; A. Mittal[1]; I. Martos-Repath[1]; G. Jha[1]; N. Mirchandani[1]; D. Das[1]; M. Onabajo[1]; A. Shrivastava[1]; S. Cash[2]; N. Sun*[1]

1. Northeastern University, Electrical Engineering, USA
2. Harvard Medical School, Department of Neurology, USA

Ultra-compact wireless implantable medical devices are in great demand for healthcare applications, in particular for neural recording and stimulation. Current implantable technologies based on miniaturized micro-coils suffer from low wireless power transfer efficiency (PTE) and are not always compliant with the specific absorption rate imposed by the Federal Communications

Commission. Moreover, current implantable devices are reliant on differential recording of voltage or current across space and require direct contact between electrode and tissue. Here, we show the first ultra-compact dual-band smart nanoelectromechanical systems magnetoelectric (ME) antenna with a size of 250×174 μm^2 that can efficiently perform wireless energy harvesting and sense ultra-small magnetic fields. The proposed ME antenna has a wireless PTE 1~2 orders of magnitude higher than any other reported miniaturized micro-coil, allowing the wireless IMDs to be compliant with the SAR limit. Furthermore, the antenna's magnetic field detectivity of 300~500pT allows the IMDs to record neural magnetic fields.

S15: Advanced Microelectronics

Memristors and Neuromorphic Computing

Room: Magnolia B/C

Session Chairs: Matthew Brahlek, Oak Ridge National Lab; Yingge Du, PNNL

10:00 AM

(EMA-133-2022) Effects of Defects and Interface on Interface-type Forming-free Memristors

A. Chen*[1]

1. Los Alamos National Lab, USA

Memristors with excellent scalability have the potential to revolutionize not only the field of information storage but also neuromorphic computing. Conventional metal oxides have been widely used as resistive switching materials in memristors. Defects such as oxygen vacancy and interface play critical roles in filamentary-type resistive switching (RS) devices. In this talk, I will discuss the role of defects such as oxygen vacancy and cation deficiency and interface on switching behavior in forming-free memristors.

10:15 AM

(EMA-134-2022) Microstructural and switching dynamics studies in VO2 devices

H. Yu*[1]; S. Ramanathan[1]

1. Purdue University-west lafyette, Materials Engineering, USA

The metal-insulator transition (MIT) in VO_2 can be triggered by applying heat, electric field, or strain fields, changing the resistivity of VO_2 by several orders of magnitude. It has also been reported that the MIT of VO_2 can occur in mere nanoseconds under an electric field. These properties of VO_2 have led to the development of selectors, fast switches, oscillator, and neuromorphic devices. Most research on VO_2 devices has been focused on improving the performance at the single device level. Yet, it is also very important to understand the behavior of VO_2 switching dynamics and their interactions in interconnected circuits. Thus, a circuit with two VO_2 vertical devices connected in series is studied as an example. Two step switching behavior is found when both devices are kept at room temperature. Next, we systematically vary the temperature of one device interconnected to another at room temperature and map the dynamics of the phase transition. In this presentation, we will discuss the temperature dependent XRD phase evolution of the tetragonal phase and its correlation to the electrical switching characteristics. We will also discuss the growth of high quality polycrystalline VO_2 films on various technologically relevant substrates such as Si and ITO that is of great interest to the eventual integration of Mott materials in crossbar arrays for BEOL-compatible CMOS platforms.

10:30 AM

(EMA-135-2022) Non-volatile Charge Configuration Memory devices for use in cryocomputing environment

A. Mraz*[1]; R. Venturini[1]; M. Diego[2]; A. Kranjec[1]; D. Svetin[1]; Y. Gerasimenko[3]; V. Sever[1]; I. Mihailovic[4]; J. Ravnik[5]; I. Vaskivskyi[1]; M. D'Antuono[6]; D. Stornaiulo[6]; F. Tafuri[6]; D. Kazazis[5]; Y. Ekinci[5]; V. Kabanov[1]; D. Mihailovic[1]

1. Jozef Stefan Institute, F7, Slovenia
2. Claude Bernard University Lyon 1, France
3. University of Regensburg, Germany
4. ETH Zurich, Switzerland
5. Paul Scherrer Institut, Switzerland
6. University of Naples Federico II, Italy

Cryocomputers present an alternative to classical computer technologies, possibly surpassing classical computers in both performance and efficiency. However, their progress is hindered by a lack of a suitable memory device, which would be fast, energy efficient, non-volatile and would operate at cryogenic temperatures. Here we present a conceptually unique Charge Configuration Memory (CCM) device that satisfies all the criteria stated above and is also very straightforward in its design meaning it can be upscaled into bigger memory systems. We present a non-volatile CCM device based on electrical switching between different charge configuration states in a transition metal dichalcogenide 1T-TaS_2. We show the basic current-voltage characteristics of the device, low write energies (2.2 fJ/bit), ultrafast switching (16 ps FWHM) and good endurance (>10^6 cycles). We expose the electronic landscape of the CCM device during device's operation using a scanning tunnelling microscope (STM), which gives valuable insight into the non-volatility of the CCM device. We examine the possibility of integrating the CCM device into a superconducting Single Flux Quantum (SFQ) system by using a superconducting buffer element called a nanocryotron. We present the time dynamics and current-voltage characteristics of such a hybrid device, which show the viability of this approach and its potential for future research.

10:45 AM

(EMA-136-2022) Achieving High Performance Resistive Switching Using Ionic Thin Films

M. Xiao*[1]; C. Yun[1]; M. Elshenawy[1]; Z. Sun[1]; M. Wells[1]; M. Hellenbrand[1]; J. MacManus-Driscoll[2]

1. University of Cambridge, United Kingdom
2. University of Cambridge, Dept. of Materials Science, United Kingdom

Resistive switching (RS) materials, often called memristors, are promising candidates for next-generation non-volatile memory and neuromorphic computing applications. Positive attributes include simplicity, compatibility with conventional semiconductor processes, and the potential for 3D and scaling. For memory applications, achieving all optimized properties together of very long retention, fast switching time, endurance, uniformity, and scaling is challenging. In this talk, we revisit the challenge of achieving simultaneous performance optimization and show how tuning the transport properties in the ionic material is important to this end. With the introduction of the ionic materials, we demonstrated pronounced resistive switching performance at low voltages without high voltage electroforming, strong endurance (no change in resistance states after >1E7 cycles), stable multilevel switching for more than 32 levels, and fast switching speed of less than 20ns.

11:00 AM

(EMA-137-2022) Memristive Materials and Devices for Neuromorphic Computing (Invited)

J. Yang*[1]

1. University of Southern California, Electrical and Computer Engineering Department, USA

Memristive devices have become a promising candidate to enable efficient computing for the big data and IoT era. Such computing can be implemented on a Resistive Neural Network with memristive synapses and neurons or a Capacitive Neural Network with memcapacitive synapses and neurons. I will first briefly introduce the promises and challenges of memristive materials and devices for such applications and then discuss examples with different levels of bio-inspiration: first, deep learning accelerators with supervised online learning; second, neuromorphic computing for pattern classification with unsupervised learning; last, other computing applications, such as reinforcement learning for decision making, artificial nociceptors for robotics, provable key destruction and true random number generators for cybersecurity.

11:30 AM

(EMA-138-2022) A Dynamical Compact Model of Diffusive and Drift Memris- tors for Neuromorphic Computing

Y. Zhuo*[1]

1. University of Southern California, ECE, USA

Different from non-volatile memory applications, neuromorphic computing applications utilize not only the static conductance states but also the switching dynamics for computing, which calls for compact dynamical models of memristive devices. In this work, we present a generalized model to simulate diffusive and drift memristors with the same set of equations, which have been used to reproduce experimental results faithfully. We chose the diffusive memristor as the basis for our generalized model because it possesses complex dynamical properties that are difficult to model efficiently. A data set from statistical measurements on SiO2:Ag diffusive memristors was collected to verify the validity of the general model. As an application example, spike-timing-dependent plasticity was demonstrated with an artificial synapse consisting of a diffusive memristor and a drift memristor, both modeled with this comprehensive compact model.

11:45 AM

(EMA-139-2022) Electronic transport mechanisms in hydrogenated perovskite nickelate memristors

Q. Wang*[1]; Z. Zhang[2]; S. Ramanathan[1]

1. Purdue University, Materials Engineering, USA
2. Xi'an Jiaotong University, China

Perovskite rare-earth nickelates, as an emergent class of corelated complex oxides, display metal-insulator-transition with the conductivity modulation of 10^8 orders of magnitude by electron doping. During the process of palladium (Pd) assisted hydrogenation of nickelate thin films, hydrogen molecules with be split into protons and electrons at the triple phase boundary of Pd/H_2/nickelate. The electrons will reduce Ni^{3+} to Ni^{2+} while the protons remain in the lattice interstitial sites. Electron doping opens a wide energy band gap of nickelates which significantly modifies the conducting mechanism of the as doped nickelate, simultaneously generating a Schottky barrier at the metal-oxide interface. In this work, we will present an asymmetrical design of two-terminal devices fabricated on $SmNiO_3$ and $NdNiO_3$ thin films. The device has Pd at one side and gold at the other, and the gap between them are aligned by e-beam lithography down to 100nm. The charge carrier transport mechanisms are analyzed by investigating the current-voltage relationships as well as temperature dependent resistance change. The competing conducting mechanisms of thermionic emission over the Schottky barrier and space-charge-limited current (SCLC) conduction will be discussed. The systematic study of carrier transport physics will provide further insight into neuromorphic computing design and applications with such devices.

12:00 PM

(EMA-140-2022) Cold Sintering and Cold Flow of $MAPbBr_3$ for Large-Area Radiation Detectors

M. Tolchin*[1]; S. Lowum[1]; I. Dursun[2]; N. C. Giebink[2]; J. Maria[1]

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

$MAPbBr_3$ is a hybrid organic-inorganic perovskite semiconductor with compelling photovoltaic properties. As demands for $MAPbBr_3$ move beyond single crystal or thin film embodiments, managing microstructure becomes increasingly important. Given $MAPbBr_3$'s counterion selectivity to lead, this material affords plasticity and solvation abilities excellent for bulk processing. Cold flow (CF) and particularly, cold sintering process (CSP), are promising ways to make large, high-throughput assemblies at ultra-low temperatures. Herein, $MAPbBr_3$ crystals prepared via inverse temperature crystallization (ITC) can be densified using CF and CSP into ceramic monoliths with densities near the 100% theoretical limit. The process is scalable from mm to several cm, drawing interest for bulk polycrystalline radiation detectors which require thick slabs of bulk material. We show densification and key morphological responses by varying pressure and temperature and assigning liquid and crystalline transport phases in CSP. To connect microstructure to electrical performance, we present radiation test results including photoelectric response upon hard x-ray exposure and time of flight i-v analysis upon super bandgap laser exposure for carrier mobility. These microstructure-property trends will build our investigation into densification modes that can produce bulk $MAPbBr_3$ ceramics that are viable, large-area radiation detectors.

Complex Oxides for Device Applications

Room: Magnolia B/C

Session Chairs: Jian Liu, University of Tennessee; Anand Bhattacharya, Argonne National Laboratory

2:00 PM

(EMA-193-2022) Electrode Chemistry Influence on Hafnium Zirconium Oxide Ferroelectric Performance (Invited)

J. Ihlefeld*[1]; S. Fields[1]; S. W. Smith[2]; S. T. Jaszewski[1]; M. D. Henry[3]; S. L. Wolfley[3]; P. J. Ryan[4]; C. Fancher[5]; G. Esteves[3]; P. S. Davids[3]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. Radiant Technologies, USA
3. Sandia National Laboratories, USA
4. Argonne National Lab, Advanced Photon Source, USA
5. Oak Ridge National Lab, USA

Hafnium oxide-based 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 utilizing pyroelectric responses, among others. In this presentation, we will highlight the joint activities between the University of Virginia and Sandia National Labs to gain an understanding of electrode chemistry impacts to performance of this exciting material. The electrode materials to be highlighted cover several different classes spanning noble metals (Pt), metal nitrides (TaN), elemental moderate work function metals (W), and conductive oxides (RuO_2). We will discuss how phase constitution is impacted by the electrodes chosen and how wake-up and fatigue phenomena are dependent upon the electrode chemistry. We will

show that these effects are, in-part, due to phase transformations for some electrodes (e.g. Pt, TaN, and W electrodes), but that domain pinning due to charge injection dominates the fatigue process for others (e.g. RuO_2). These phenomena will be discussed in the context of oxygen vacancies and their impact on ferroelectric hafnia performance.

2:30 PM

(EMA-194-2022) Development of sputtered gate oxides for wide bandgap semiconductors devices

L. Shvilberg*[1]; T. MIMURA[1]; J. J. Wierer[3]; E. A. Paisley[2]; J. Ihlefeld[1]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. Sandia National Laboratories, USA
3. North Carolina State University, Department of Electrical and Computer Engineering, USA

Wide bandgap semiconductors, including SiC and GaN, are replacing Si-based technology in power switching applications because of their ability to perform efficiently under extreme conditions. A challenge facing specific classes of SiC and GaN devices is development of a robust dielectric insulating layer that is chemically and thermally compatible with the semiconductor. In gate dielectric applications, additional requirements include sufficient band offsets and low leakage currents and interface state densities. Oxides, such as MgO, CaO, and (Mg,Ca)O, hold promise as they have been shown to meet many of these requirements in epitaxial films synthesized by molecular-beam epitaxy, pulsed laser deposition, and atomic layer deposition. Large area growth with low impurity content and smooth growth surfaces are a remaining obstacle. This talk will present results showing epitaxial growth of MgO and CaO by RF magnetron sputtering on GaN. 4-circle X-ray diffraction data will be shown to demonstrate epitaxial growth for each material. Initial electrical characterization shows leakage currents far lower than achieved in ALD counterparts and clear depletion and accumulation of charge in metal-oxide-semiconductor devices.

2:45 PM

(EMA-195-2022) Self-biased electric control of magnetism at room temperature in single layer composite films, harnessing the interplay of anitferromagnetism, ferrimagnetism and ferroelectricity (Invited)

J. MacManus-Driscoll*[1]

1. University of Cambridge, Dept. of Materials Science, United Kingdom

In this work, we used a new vertically aligned nanocomposite (VAN) 3-1 system to overcome the long-standing challenges of unwanted leakage and for the need of magnetic field biasing to achieve a magnetoelectric effect at room temperature magnetoelectrics. To this end, we design and grow thin films of $Na_{0.5}Bi_{0.5}TiO_3$(matrix)-NiO(column-shell)-$NiFe_2O_4$(column)-core. The system shows excellent self-biased magnetoelectric properties at room temperature. The measured ME coefficient, α_{33}= 1.38×10^{-9} s m^{-1}, is large enough to switch the magnetic anisotropy from the easy-axis (K_{eff} = 0.91×10^4) to the easy-plane (K_{eff} = -1.65×10^4). Three key effects led to the notable result - a large reduction of the leakage, strong exchange coupling between the antiferromagnetic NiO and ferrimagnetic $NiFe_2O_4$, producing a large exchange bias effect, eliminating the need for magnetic field application for achieving ME; and an additional magnetoelastic effect from NiO, which adds to that already present in the $NiFe_2O_4$ columns, to enable a stronger ME effect.

3:15 PM

(EMA-196-2022) Plasmon Induced Hot Electron in Metal Nanostructures for Enhancing Performance of Photodetectors

S. Kunwar*[1]; A. Chen[1]

1. Los Alamos National Lab, USA

The strong localized surface plasmon resonance (LSPR) induced by the incident electromagnetic radiation in noble metallic nanoparticles have attracted significant attention in the field of energy and environment, microscopy, medicines, photonics, sensing and optoelectronics. The relaxation of LSPR induces radiative (scattering) and non-radiative (absorption and hot-electron injection) effects, which offers a facile route to enhance the performance of optoelectronic devices such as photodetectors. Herein, we explore the significance of various plasmonic NPs in photodetectors in combination with the semiconductor photoactive layers. The hybrid device architectures are initially optimized based on the structure, configuration and arrangement of metal NPs and photoactive layers and then subsequently the enhanced photoresponse in the ultra-violet, visible and near-infrared regime has been demonstrated. In comparison to the pristine devices, the plasmon enhanced photodetectors clearly show significant improvement in the photoresponsivity, detectivity and external quantum efficiency in the broad range of electromagnetic spectrum. At the same time, the structural and elemental tunability in the plasmonic NPs offer efficient injection of hot electrons into the semiconductor's conduction band, longer carrier lifetime as well as altered Schottky barrier height at the interface.

4:00 PM

(EMA-197-2022) Unit-cell-scale ferroelectricity : Flat band breaks the 100-year-old myth of necessitating domains (Invited)

J. Lee*[1]

1. Ulsan National Institute of Science & Technology, Republic of Korea

Since ferroelectricity is a collective phenomenon necessitating thousands of atoms' simultaneous displacement, it's been believed since it's discovery in 1920 that at least finite-sized domains (10~100nm) are required to stabilize and switch the ferroelectric dipole moments. Here, we show that we can break the 100-years myth if we introduce flat-band theory in the history of ferroelectricity. As flat band has been known to induce intrinsic local states and to cause very unusual phenomena such as graphene superconductivity and electron lattices, we, for the first time, show that flat band in ferroelectricity induces intrinsic local dipoles of unit-cell scale of a few angstroms. These intrinsic local dipoles are individually stable and switchable, now one does not need the formation of the conventional domains for the dipole switching. We can directly switch the unit-cell-scale dipoles and finally pave a way to achieve ultimate-density ferroelectric devices.

4:30 PM

(EMA-198-2022) Extreme tensile strain states in complex oxide membranes (Invited)

S. Hong*[1]

1. UC Davis, USA

A defining feature of emergent phenomena in complex oxides is the competition and cooperation between ground states. In manganites the balance between metallic and insulating phases can be tuned by the lattice; extending the range of lattice control would enhance the ability to access other phases. Freestanding complex oxide membranes provide unique opportunities to realize previously unobserved strain-induced responses. Oxide membranes can be mechanically coupled to an external platform without an epitaxial relationship, of which strain states and symmetries can be freely chosen by design. Moreover, the critical fracture strain is often greatly enhanced for small materials length scales, allowing tensile strain states larger than the typical values ceramics withstand. Here

we stabilize uniform tensile strain in $La_{0.7}Ca_{0.3}MnO_3$ membranes, exceeding 8% uniaxially and 5% biaxially. Uniaxial and biaxial strain suppresses the ferromagnetic metal at distinctly different strain values, inducing an insulator that can be extinguished by magnetic field. This highly-tunable strained membrane approach provides a broad opportunity to design and manipulate correlated electron states.

Friday, January 21, 2022

S4: Complex Oxide Thin Films and Heterostructures: From Synthesis to Strain/ Interface-engineered Emergent Properties

Strain, Microstructures and Functionality Tuning

Room: Orange A

Session Chair: Sangmoon Yoon, Oak Ridge National Lab

8:30 AM

(EMA-199-2022) Engineering Metastable 4d and 5d Complex Oxide Films for Emergent Interfacial Phenomena by Hybrid Molecular Beam Epitaxy (Invited)

R. B. Comes*[1]

1. Auburn University, Dept. of Physics, USA

Complex oxides comprised of 4d and 5d cations exhibit a host of intriguing and useful properties for new technologies due to their enhanced spin-orbit coupling and variety of valence states. Engineering these materials to produce metastable charge states such as a $4d^1$ or $5d^1$ state can be a powerful tool to produce new interfacial properties in complex oxides. Through the use of hybrid molecular beam epitaxy (MBE), we are able to engineer these materials down to the atomic level so that interfaces between two different materials can be controlled to produce desirable properties. In this talk I will show how we can optimize these systems using in situ X-ray photoelectron spectroscopy techniques to understand the film growth process and resulting electronic properties. I will show how hybrid MBE can enable synthesis of hard to grow materials using metalorganic precursors, including $SrNbO_3$, $SrTaO_3$ and $SrHfO_3$. $SrHfO_3$ is employed as a capping layer to preserve the metastable electronic configuration of $SrNbO_3$ and $SrTaO_3$. These materials are coupled into heterostructures for future use as 2-dimensional electron gases (2DEGs) with high electron mobility. $SrNbO_3$ films grown on $BaSnO_3$ are examined as a means of increasing the carrier concentration in $BaSnO_3$. Meanwhile, buried $SrTaO_3$ layers are examined for their potential as spin-orbit coupled 2DEGs.

9:00 AM

(EMA-200-2022) Examination of Biaxial Stresses Produced by the Clamping Effect in HZO Thin Films (Invited)

S. Fields*[1]; T. Cai[3]; S. T. Jaszewski[2]; B. Sheldon[3]; J. Ihlefeld[1]

1. University of Virginia, Department of Materials Science and Engineering, USA
2. University of Virginia, Materials Science and Engineering, USA
3. Brown University, School of Engineering, USA

The biaxial stresses yielded by the electrode clamping effect are quantified using $sin^2(psi)$ analyses of diffraction patterns measured on 20 nm thick $Hf_{0.5}Zr_{0.5}O_2$ (HZO) films processed on TaN bottom electrodes with and without top TaN electrodes. The samples both demonstrate tensile biaxial stress following processing and the clamping effect is shown to yield a two-fold increase (1.6 GPa) in the stress magnitude. Wafer flexure-based stress measurements are also carried out on the samples before and after each processing step. While TaN electrode deposition produces compressive biaxial stress, PE-ALD growth of the HZO and annealing of the completed film stacks produces tensile biaxial stress. Flexure measurements reveal that the clamping effect produces 0.3 GPa in the film stack. SEM and leakage current measurements reveal no clear dependence of grain size or defect density on the top electrode presence. X-ray Reflectivity measurements of HZO films that were left unannealed and annealed with and without TaN top electrodes reveal that the tensile biaxial stress is yielded through a 4% densification of the HZO during crystallization, however the densification is not dependent on the presence of the top electrode. To further examine the clamping effect mechanism, temperature-resolved flexure and XRD measurements are carried on samples with and without top electrodes during heating and cooling.

9:15 AM

(EMA-201-2022) A thin defective layer formation in yttria-stabilized zirconia and its ferromagnetism

S. Ryu*[1]; D. Cho[1]; J. Park[2]; J. Lee[2]; T. Hong[3]; M. Byeon[3]; H. Jeen[1]

1. Pusan National University, Republic of Korea
2. Korea Atomic Energy Research Institute, Korea Multi-Purpose Accelerator Complex, Republic of Korea
3. Korea Basic Science Institute, Busan Center, Republic of Korea

Ferromagnetism in oxygen-deficient ZrO_2 has been reported. In this work, the nitrogen ion beam was irradiated to YSZ single crystals. To identify penetration depth of ion beam, simulation was proceeded. Defective thin layer was formed in the YSZ by ion beam. The thickness of defective layer was similar to the simulation, and the increase of the lattice constant was observed by x-ray diffraction. In addition, nitrogen depth profiling was obtained by secondary ion mass spectrometry (SIMS). Oxygen vacancy formation is evidenced by EDS/STEM analysis. Interestingly, ferromagnetic hysteresis is observed in the irradiated YSZs at room temperature. To find origin of such ferromagnetic behavior, we thermally created oxygen vacancies in YSZ and observed ferromagnetic behavior. We'll argue the origin of ferromagnetism in the defective layer.

9:30 AM

(EMA-202-2022) Strain induced negative thermal expansion in molecular beam epitaxy grown $LaVO_3$ thin films

K. Noordhoek*[1]; A. R. Mazza[1]; J. M. Lapano[1]; T. Z. Ward[1]; R. Engel-Herbert[2]; V. R. Cooper[1]; Y. Cao[3]; M. Brahlek[1]

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Pennsylvania State University, Department of Materials Science and Engineering, USA
3. Argonne National Lab, Materials Science Division, USA

Understanding the complex role that crystal structure plays in modifying electrical and magnetic properties of a material is critical for designing and controlling functional phenomena. In bulk, the strongly correlated Mott insulating RVO_3 system (where R = rare earth) is highly sensitive to chemical pressure, which tunes the transition temperatures for both orbital and spin ordering by controlling a structural instability. Here, we show that epitaxial strain can be effectively used to control the character of the structural phase transition in $LaVO_3$ films grown by hybrid molecular beam epitaxy. At highly compressive strains the films exhibit a large first-order phase transition, while at moderate compressive and tensile strains the phase transition is nearly quenched. Furthermore, low strains give rise to an anomalous negative thermal expansion, which is completely absent in the bulk phase diagram. This not only demonstrates the important role of structure on complex properties, but also shows the unique nature of epitaxial strain to tune properties into unexplored regimes and is an important route to unveiling and tuning hidden phenomena. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

9:45 AM

(EMA-203-2022) Effect of the strain and polar defect on dielectric, ferroelectric, and energy storage properties of epitaxial relaxor ferroelectric thin films

J. Belhadi*[1]; U. Trstenjak[2]; D. Fabijan[2]; D. Vengust[2]; N. Daneu[2]; M. Benyoussef[1]; M. El Marssi[3]; V. Bobnar[4]; M. Spreitzer[5]

1. Université de Picardie Jules Verne, France
2. Jozef Stefan Institute, Advanced Materials Department, Slovenia
3. Université de Picardie Jules Verne, LPMC, France
4. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia
5. Jozef Stefan Institute, Advanced Materials, Slovenia

Strain and polar defect engineering in oxide ferroelectric thin films have become a powerful route to control, tune, and enhance the functional properties and also create/induce new exotic properties that do not exist in bulk materials. In the present work, we report the effect of both the epitaxial strains and the polar defects created during the growth on the structural, ferroelectric, phase transitions, and energy storage properties of the prototypical relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ (PMN-xPT) thin films. By optimizing the pulsed laser deposition parameters and using dense home-made PMN-PT targets with PbO excess, high-quality PMN-PT/$SrRuO_3$ (SRO) heterostructures with different strain states were grown on high crystalline quality and single terminated $SrTiO_3$ and $REScO_3$ (RE= Dy, Gd, Sm) substrates with different unit-cell sizes. In-situ Reflection High-Energy Electron Diffraction was used to monitor the growth mode and surface quality of the SRO and PMN-PT layers during the growth. The phase, crystalline quality, and the domain structure of the as-grown films were controlled using high-resolution X-ray diffraction. The ferroelectric, dielectric, and energy storage properties of the heterostructures were investigated and correlated to the growth conditions, strain state and polar defects.

Characterizations of Strain, Defects, and Interfaces

Room: Orange A

Session Chair: Ryan Comes, Auburn University

10:30 AM

(EMA-243-2022) Understanding interfacial stabilization and disorder for highly metallic epitaxial delafossites (Invited)

S. Yoon*[1]; J. Ok[1]; A. Huon[1]; T. Ichiba[1]; M. Yoon[1]; S. Yeom[2]; F. R. Reboredo[1]; A. R. Lupini[1]; H. Lee[1]

1. Oak Ridge National Lab, USA
2. University of Tennessee, USA

Metallic delafossite oxides have attracted considerable attention for their natural heterostructures, highlighting the combination of nearly free electrons and band/Mott insulating states. Such unique electronic properties have motivated recent attempts to grow delafossite thin films or heterostructures. The epitaxial growth of metallic delafossites not only provides a route to utilize their diverse properties in future devices but also enables the design of artificially structured delafossite metals in which new quantum phenomena may emerge. Despite extensive research interests, the field is still in its infancy. In this talk, we will show our research effort to synthesize high-quality epitaxial delafossites, and atomic-scale phenomena occurring at the interfaces between delafossites and between delafossite and substrate. We will show our observations on the significant interlayer diffusion between delafossites, and a way to control the interface symmetry by utilizing this phenomenon to stabilize the nucleation of metallic delafossites. Furthermore, we found that the surface termination is critical to control structural twins formed in epitaxial delafossites, which determines low-temperature transport behavior. Finally, we will show our discovery to synthesize a flat delafossite-buffered substrate with an extremely sharp interface using a hybrid solid-state reaction.

11:00 AM

(EMA-244-2022) Autonomous exploration of nanoscale strain with active learning in 4D-STEM

K. M. Roccapriore*[1]; M. Ziatdinov[1]; O. Dyck[1]; S. Kalinin[1]

1. Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, USA

Recent developments in the scanning transmission electron microscope (STEM) have enabled the quantification of strain in nanoscale objects, particularly with pixelated or direct electron detectors. While aberration corrected STEM has provided atomic resolution to map atomic coordinates and therefore deduce local strain, this requires precise orientation relative to the electron beam. On the other hand, with nano beam electron diffraction (NBED) in the form of 4D-STEM, nanoscale strain can be mapped for any orientation, where diffraction patterns are recorded at every probe position and strain is then calculated from the 4D data. Knowledge of where to probe strain in materials based on structural information, e.g., annular dark field (ADF) images, can be elusive. The ADF contains information about other details of the system, such as electronic properties or strain, however, this relationship is not well-defined. We propose active learning on the microscope that correlates the structural information obtained in the ADF to the diffraction patterns in NBED to guide the subsequent points in space to explore. Autonomous experimentation of probing strain is demonstrated in a variety of materials in the STEM based on structural image feedback using a deep kernel learning approach.

11:15 AM

(EMA-245-2022) Structural evolution of oxide heterostructures: Thermal, optical, and electronic characterization via ultrafast spectroscopic methods

J. Tomko*[1]; S. Hoseini Makrem[2]; E. Hogland[2]; R. Ramesh[3]; P. E. Hopkins[1]

1. University of Virginia, Mechanical and Aerospace Engineering, USA
2. University of Virginia, Materials Science and Engineering, USA
3. UCBerkeley, MSE/Physics, USA

As individual layer thicknesses approach that of a single unit cell, superlattices and heterostructures can remarkably evolve from a material described by an 'average' of its constituents to a material instead described by a single emergent and coherent structure. The interfacial coupling that gives rise to this structural evolution has been intensely investigated for unique material design and property engineering, including 2DEG formation and control of metal-insulator transformations. However, a detailed description of the underlying vibrational and thermal properties across this structural evolution remains lacking. In this work, we perform a series of ultrafast laser spectroscopy methods to demonstrate the emergence of a dynamic property evolution that occurs in-tandem with the observed structural evolution of oxide superlattices and heterostructures. In other words, we demonstrate a series of structure-property relationships in superlattices with greatly reduced periodicity that arise solely due to interfacial structural coupling/coherence. Specifically, we investigate the electronic polarizability, phonon scattering rates, and optical absorbance of oxide superlattices with varying degrees of coherence; these results are compared to trends in thermal conductivity across the structural transition and advanced STEM/EELS characterization.

11:30 AM

(EMA-246-2022) Cooling rate dependence of structure and composition in (Nd,Li)TiO3/SrTiO3 thin films deposited by PLD

E. Farghadany*[1]; N. Bagués[3]; H. B. Smith[1]; B. Powers Beggs[2]; D. W. McComb[3]; A. Sehirlioglu[4]

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

A-site deficient perovskite structure is commonly studied for a variety of applications. (RE,Li,vacancy)TiO3 is a good candidate for Li transport. Processing of this material as a single crystal thin film eliminates the grain boundaries which act as barriers for diffusivity of the species. Chemical and structural characterization of the thin film system is critical as the thin film crystals are grown under non-equilibrium conditions and provide a path to tailor the properties of the material through processing control. A processing parameter that is often ignored is the cooling rate after deposition. In this study, films that were grown in the optimized monolayer growth regime by pulsed laser deposition (PLD), were cooled down by a variety of cooling rates. The relationship between surface morphology (characterized by AFM), and cross-sectional structure (characterized by HR-TEM) and composition (characterized by ToF-SIMS) was shown. Two different regimes were observed with varying defect characteristics, intermixing profiles and surface morphologies as a result of the competition between the stored elastic energy and the thermal stress.

11:45 AM

(EMA-247-2022) Calorimetric and Thermogravitational Characterization of $Y_{0.2}La_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ Solid Solutions

C. Skidmore*[1]; G. N. Kotsonis[2]; J. Maria[2]

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

The rare earth-based high-entropy oxide (HEO) $Y_{0.2}La_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ (F1) has become an insightful prototype for studying fluorite-derived HEOs with significant oxygen deficiency. F1 can be synthesized by solid-state reaction, physical vapor deposition, or solution precipitation, but the microstructure and crystalline symmetry varies depending on choice of synthesis technique and synthesis kinetics. Bulk F1 specimens typically exhibit oxygen sublattice ordering indicative of bixbyite-type ordering within a fluorite matrix, but nanocrystals made by solution precipitation appear to take the higher-symmetry fluorite structure. Additionally, the net Pr valence and optical band gap depend on oxygen chemical potential during synthesis or heat treatment. This talk discusses bulk synthesis of F1, including a calorimetric investigation during the solution formation reaction. With well-prepared powders, dense F1 ceramics can be sintered readily at 1400 °C. Calorimetry indicates a peak endotherm near 1100 °C. Combined calorimetry and thermogravitational analysis reveal two low-temperature reactions that likely correspond to evaporation of adsorbed solvent from milling and the conversion of La or Sm hydroxide to oxide prior to F1 formation. We also present a Kissinger analysis of calorimetry data to approximate the activation energy for solution formation.

12:00 PM

(EMA-248-2022) Aqueous chemical deposition of K0.5Na0.5NbO3 ferroelectric thin films

A. Z. Mohammed*[1]; S. R. Burns[2]

1. University of calgary, Chemistry, Canada
2. University of Calgary, Canada

K0.5Na0.5NbO3 (KNN) is a lead-free material often lauded for its piezoelectric properties. It is suitable for a wide variety of applications, such as sensors, actuators, and ultrasonic devices. Although the material has been extensively studied in bulk ceramic forms, thin films are less well understood. Furthermore, KNN films have not been adapted in industrial settings due to difficulties in synthesizing high quality samples with high throughput. The most promising fabrication approaches are chemical solution deposition (CSD) techniques which rely on hazardous organic solvents (2-methoxyethanol). In our approach, we synthesize aqueous solutions at room temperature derived from commercially available niobium, sodium and potassium precursors. This technique allows a precise control of stoichiometry, with which we can optimize the functional properties of our films. Moreover, this simple wet chemistry fabrication process is not as energy intensive, expensive or complex as most thin film deposition techniques. The literature indicates doping with lithium and manganese is promising for improving the piezoelectric properties of KNN thin films. To this end, our future work will allow us to explore the possibility of adding such dopants through our environmentally conscious approach.

Controlled Synthesis of Lateral and Vertical Heteroepitaxial Thin Films and Nanocomposites III

Room: Orange A
Session Chair: Aiping Chen, Los Alamos National Lab

2:00 PM

(EMA-259-2022) Strain induced magnetism in $PdCoO_2$ (Invited)

M. Brahlek*[1]

1. Oak Ridge National Lab, USA

Of particular interest to the next generation of electronic materials are the strongly correlated transition metal oxides where a variety of unexpected and unpredictable electronic phases emerge. The ABO_2 metallic delafossites specifically exhibit novel properties such as ultra-high conductivities and associated long electron mean-free-paths as well as natural 2-dimensionality composed of localized BO_2 states and itinerant states originating from the metallic A-nets. As such, creating high-quality thin films of this motif opens new ways to induce and control functional properties. In this talk I will discuss synthesizing the archetypal metallic delafossite $PdCoO_2$ by molecular beam epitaxy, as well as recent work to induce functional properties such as magnetism in this otherwise paramagnetic system. I will further discuss the insight into the physical mechanisms that give rise to emergent long-range magnetic order, which opens new routes to design magnetism in these materials. This fundamental work is a push towards opening largely unexplored phenomena in a novel class of oxide materials. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division, and the National Quantum Information Science Research Centers.

2:30 PM

(EMA-260-2022) Superconductivity in low-valence layered nickelates (Invited)

A. S. Botana*[1]

1. Arizona State University, Physics, USA

The physics behind high-temperature superconductivity in cuprates remains a defining problem in condensed matter physics. Among the myriad approaches to addressing this problem has been the study of alternative transition metal oxides with similar structures and electron count. After a 30 year quest, a non-cuprate compound with a cuprate-like structure that exhibits superconductivity has been found: hole-doped $NdNiO_2$. Given that this material is one of the members of a larger series of layered nickelates, this result opens up the possibility of a new family of unconventional superconductors. By means of first-principles calculations, we have analyzed the similarities and differences between this family of low-valence planar nickelates and cuprates. Even though these nickel oxide materials possess a combination of traits that are widely considered as crucial ingredients for superconductivity in cuprates (a square-planar

nature, combined with the appropriate 3d-electron count, and a large orbital polarization) they also exhibit some important differences (a larger p-d energy splitting, and lack of magnetism in the parent compounds). Our results show that low-valence layered nickelates offer a new way of interrogating the cuprate phase diagram and are singularly promising candidates for unconventional superconductivity.

2:45 PM

(EMA-261-2022) Approach to the practical magnetoelectrics with the vertically aligned nanocomposites (Invited)

R. Wu*[1]; S. Cho[1]; T. Maity[1]; D. Zhang[2]; A. Kursumovic[1]; P. Lu[3]; H. Wang[4]; J. MacManus-Driscoll[5]

1. University of Cambridge, United Kingdom
2. Purdue University, Materials Engineering, USA
3. Sandia National Laboratories, USA
4. Purdue University, School of Materials Engineering, USA
5. University of Cambridge, Dept. of Materials Science, United Kingdom

Magnetoelectric (ME) materials have very broad prospects in next-generation memory devices. However, the practical application of ME films is still challenged by many factors, such as the substrate clamping, the leakage, and the bias field. We have taken the following three measures to address these problems. First, we adopted a vertically aligned nanocomposite (VAN) structure instead of the traditional multilayer structure to overcome the substrate clamping effect and achieve an efficient strain coupling. Secondly, we chose the less leaky $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) instead of $BiFeO_3$ as the ferroelectric matrix. A p-n junction formed at the film-substrate interface, which further suppressed the vertical leakage current in the composite film. The low leakage enables the in-situ electric field control of magnetic properties in the ultra-thin multiferroic composite film in a large scale. In the NBT -$CoFe_2O_4$ VAN, the obtained ME coefficient is as high as 1.32×10^{-9} s m^{-1}. Finally, we introduced the antiferromagnetic phase, i.e. NiO, into the traditional ferrimagnetic-ferroelectric two-phase multiferroic composite film to form a three-phase NBT-NiO-$NiFe_2O_4$ VAN film, where a self-biased ME effect was achieved via the antiferromagnetic-ferromagnetic exchange coupling. These studies have paved the way to the practical application of composite multiferroic thin films in electronic devices.

3:00 PM

(EMA-262-2022) Disorder driven electronic and magnetic phases in high entropy oxide nickelates

A. R. Mazza*[1]; J. M. Lapano[1]; M. Brahlek[1]; T. Z. Ward[1]

1. Oak Ridge National Laboratory, USA

Disorder is an important aspect of correlated quantum systems - it can be used to manipulate superconductivity, magnetic ordering, and electronic structure. While synthesis of new quantum materials is generally focused on creating perfect crystals comprised of only a few elemental building blocks, we will present our recent efforts to create high quality single crystals with a high degree of configurational elemental disorder on sublattice sites. Using the ABO_3 nickelates as a test case, the role of extreme A-site cation size variance is explored. We grow $(Y_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}Gd_{0.2})NiO_3$ whose parent ternary oxides each have a large range of functional and structural phase transition temperatures. The metal to insulator transition - as measured by resistivity - and magnetic ordering temperatures (T_N) - as measured by resonant elastic x-ray scattering - are found to be strongly influenced by cation variance in these systems. These results suggest cation variance can be a critical order parameter in the design of correlated oxides, and that this parameter can be tuned using entropy-assisted synthesis to create multicomponent sublattices.

3:15 PM

(EMA-263-2022) Infrared optoelectronic and magneto-optic properties in Gd-doped CdO

A. Cleri*[1]; J. Murphy[2]; J. R. Schrecengost[2]; N. C. Giebink[2]; J. Maria[1]

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

CdO is one of the most promising low-loss infrared (IR) plasmonic materials to date. Incorporation of a donor dopant such as Y, In, or F has demonstrated tunable carrier concentration between 10^{19}-10^{21} cm^{-3}, corresponding to mid-IR plasmonic modal frequencies. In addition, high-power impulse magnetron sputtering (HiPIMS) consistently produces heteroepitaxial films with high mobilities between 300-500 cm^2/V-s, minimizing optical losses. We have shown how manipulating donor and acceptor defect chemistry through controlling deposition and post-processing conditions enables one to engineer epsilon-near-zero (ENZ) modes spanning a broad range of the mid- to near-IR (1650-5325 cm^{-1}). While we have largely explored light confinement in CdO via electron oscillations, we now aim to further manipulate light through magnetism by Gd doping to create a dilute magnetic semiconductor. In this presentation, we show the excellent structural and morphological properties of Gd-doped CdO across a broad doping range, enabling fine permittivity control with ENZ behavior spanning the mid- to near-IR. Further we will explore magneto-optic properties through Faraday rotation measurements and assess the effect of the ENZ condition on these properties.

S5: Mesoscale Phenomena in Ferroic Nanostructures: From Patterns to Functionalities

Applications involving Electronic, Magnetic, Thermal, Optical, and Electrochemical Functionalities

Room: Cypress B

Session Chair: Hemaprabha Elangovan, Technion Israel Institute of Technology

8:30 AM

(EMA-204-2022) Unexpected Temperature-Dependence Mesoscale Polarization in Ferroelectrics

Y. Ivry*[1]

1. Technion - Israel Institute of Technology, Israel

Ferroelectricity is a unique functional platform that comprises collective electron and dipole-moment behavior. The onset of ferroelectricity occurs at a temperature-driven phase transition. Hence, understanding the atomic-scale dipole-moment and mesoscale domain organization at variable temperatures is vital for revealing the fundamentals of ferroelectricity. Nevertheless, observing temperature dependence of dipoles and domains is a challenging experimental task. Here we present the atomic scale and domain scale origin of ferroelectricity by means of direct observations, using atomic-scale electron microscopy and mesoscale piezoresponse and conductivity microscopy with in-situ temperature variation. Our results help realize the phase transition mechanism in $BaTiO_3$ as well as the attractive polarization-based photoconductivity in $MAPbI_3$.

8:45 AM

(EMA-205-2022) Enhanced ferroelectricity in $Hf_{0.5}Zr_{0.5}O_2$ film using oxygen-providing electrodes (Invited)

M. Park*[1]; K. Yang[2]; G. Yu[2]; S. Kim[2]; D. Lee[2]; J. Park[2]; G. Park[2]

1. Seoul National University, Department of Materials Science and Engineering, Republic of Korea
2. Pusan National University, School of Materials Science and Engineering, Republic of Korea

Ferroelectricity in fluorite-structured oxides has been studied since its first report in 2011. DIfferent from the conventional ferroelectric, this emerging binary ferroelectric material is compatible with the conventional semiconductor technology based on its characteristic physical scalability. However, such thin films suffer from the defective interfacial layer, which is the origin of the frequently observed 'wake-up effect' accompanied by pristine distortion of the polarization-electric field. The origin of the wake-up effect has been suggested to be strongly related to the charged defects and their redistribution during the repetitive polarization switching. and resulting domain wall depinning as well as local phase transformation. To prevent the wake-up effect which is not optimal for reliable electronic devices based on fluorite-structured ferroelectrics, the concentration of defects such as oxygen vacancies should be decreased. In this study, by applying suitable electrode materials, the remanent polarization of the $Hf_{0.5}Zr_{0.5}O_2$ film could be improved, and the wake-up effect could be significantly mitigated.

9:15 AM

(EMA-206-2022) Strain effect on relaxor ferroelectric domains in epitaxial PMN-PT/SRO heterostructures

M. Spreitzer*[1]; J. Belhadi[1]; U. Trstenjak[1]

1. Jozef Stefan Institute, Advanced Materials, Slovenia

Controlling the growth of complex relaxor ferroelectric thin films and understanding the relationship between biaxial strain–structural domain characteristics are desirable for designing materials with a high electromechanical response. Here, we used optimized growth parameters and target compositions to obtain epitaxial (40–45 nm) $0.67Pb(Mg_{1/3}Nb_{2/3})O_3$–$0.33PbTiO_3$/(20 nm) $SrRuO_3$ (PMN–33PT/SRO) heterostructures using pulsed-laser deposition on singly terminated $SrTiO_3$ (STO) and $ReScO_3$ (RSO) substrates with Re = Dy, Tb, Gd, Sm, and Nd. RHEED and HR-XRD analysis confirmed high-quality and single-phase thin films with smooth 2D surfaces, while HR-STEM revealed sharp interfaces and homogeneous strain further confirming the epitaxial cube-on-cube growth mode of the PMN–33PT/SRO heterostructures. The results showed that the domain structure of the PMN–33PT heterostructures is sensitive to the applied compressive strain. An evolution from a butterfly-shaped diffraction pattern for mildly strained PMN–33PT layers, which is evidence of stabilization of relaxor domains, to disc-shaped diffraction patterns for high compressive strains with a highly distorted tetragonal structure, is observed. The obtained results show that epitaxial strain engineering could serve as an effective approach for tailoring and enhancing the functional properties in relaxor ferroelectrics.

9:30 AM

(EMA-207-2022) Hafnia-based ferroelectric tunnel junctions (Invited)

B. Prasad*[1]; V. Thakare[2]; Z. Zhang[2]; A. Kalitsov[1]; T. Santos[1]; R. Ramesh[3]

1. Western Digital, USA
2. University of California, Materials Science and Engineering, USA
3. UCBerkeley, MSE/Physics, USA

High density, high-speed and low power consuming nonvolatile memories are currently being vigorously explored for use in next-generation computation, particularly due to the performance gap between the logic and memory elements of the current computational architecture. Electrically switchable spontaneous polarization of ferroelectric materials enables a robust nonvolatile memory solution. Using ultrathin films of ferroelectric materials as a tunnel barrier in metal/ferroelectric/metal trilayer structure, so-called ferroelectric tunnel junctions (FTJ), is being explored widely as a potential nonvolatile memory element. Unlike ferroelectric RAM (FeRAM), FTJ offers nondestructive readout, in addition to low operation energy and high operation speed. In this work, we have demonstrated FTJs with a very large OFF/ON resistance ratio and relatively low resistance area product (RA) with ~ 1 nm thick Zr doped HfO_2 (HZO) ferroelectric tunnel barrier. We stabilized ferroelectricity in ultrathin films of rhombohedral HZO (R-HZO) through the substrate-induced compressive strain. The resistance area product at the bias voltage (~ 300 mV) required for one-half of the zero-bias TER ratio is three orders of magnitude lower than the reported value with relatively thick ferroelectric barriers. These results set the stage for further exploration of Hafnia-based FTJs for non-volatile memory applications.

Chemistry and Physics of Ferroic Materials at Mesoscale

Room: Cypress B

Session Chair: Binod Paudel, New Mexico State University

10:30 AM

(EMA-249-2022) Multi-objective Bayesian optimization of functional materials responses for memoryand energy storage applications

A. Biswas*[1]; A. Morozovska[2]; M. Ziatdinov[3]; E. Eliseev[4]; S. Kalinin[1]

1. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
2. Institute of Physics, National Academy of Sciences of Ukraine, Ukraine
3. Oak Ridge National Laboratory, Computational Sciences and Engineering Division, USA
4. National Academy of Sciences of Ukraine, Institute for Problems of Materials Science, Ukraine

Optimization of materials performance for specific applications often requires balancing multiple aspects of materials functionality. Even, where generative physical model of material behavior is known and reliable, this often requires search over multidimensional function space to identify low-dimensional manifold corresponding to required Pareto front. Here we introduce the multi-objective Bayesian Optimization (MOBO) workflow for the ferroelectric/anti-ferroelectric performance optimization based on the numerical solution of the Ginzburg-Landau equation with electrochemical or semiconducting boundary conditions. MOBO is a low computational cost optimization tool for expensive multi-objective functions, where we update posterior Gaussian process models from prior evaluations, and then select future evaluations from maximizing an acquisition function. Using the parameters for a prototype bulk antiferroelectric ($PbZrO_3$), we first develop a physics-driven decision tree of target functions from the loop structures. Then, a physics-driven MOBO architecture is developed to build and explore Pareto-frontiers by maximizing multiple target functions jointly - e.g. energy storage and loss. This approach allows for rapid initial materials and device parameter selection for a given application and can be further expanded towards the active experiment setting.

10:45 AM

(EMA-250-2022) Exotic Dipolar Structures and Properties in Ferroelectric Superlattices (Invited)

L. W. Martin*[1]

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

We will highlight recent advances in the study of ferroelectric/dielectric superlattices such as $(PbTiO_3)_n$/$(SrTiO_3)_m$ and others wherein unit-cell-level control enables one to place various energies into competition which drives the formation of topologically

non-trivial structures including so-called polar vortices and skyrmions. We will introduce and explore a number of aspects of these systems, including: the fundamental nature of the features that can be produced and the mechanisms behind their formation, routes to tune the morphology of the emergent structures to produce both polar vortices and skyrmions with a skyrmion number of +1, observations of phase coexistence (mediated by a first-order phase transition) between such emergent, non-trivial phases and trivial ferroelectric phases, the potential for the formation of a novel multi-order-parameter state which belongs to a class of gyrotropic electrotoroidal compounds, the realization of electric-field control of such systems and concomitant order of magnitude changes in piezoelectric and nonlinear optical responses, electric-field and light susceptibilities, the potential for exotic dielectric phenomena, and much more. All told, this presentation will provide an introduction to this growing field, a dive in the latest discoveries, highlight similarities and differences with the magnetic community, and more.

11:15 AM

(EMA-251-2022) Atomic-scale electromechanical effects of individual oxygen vacancies at ferroelectric domain walls

H. Elangovan*[1]; M. Barzilay[1]; A. Hershkovitz[1]; J. Huang[2]; S. Liu[2]; S. Cohen[3]; Y. Ivry[1]

1. Technion Israel Institute of Technology, Department of Materials Engineering, Israel
2. Westlake University, China
3. Nuclear Research Centre-Negev, Israel

Oxygen vacancies at ferroelectric domain walls garner much attention in recent years because they bring in exciting charge transport amidst the highly insulating bulk (domains) as well as due to the more traditional role that they play as domain-wall pinning centers. However, (sub)atomic-scale effects of individual oxygen vacancies have remained elusive due to the challenges associated with observing and manipulating objects at this scale. Recently, we demonstrated the in situ formation of domains and domain walls along with strain and charge distribution mapping at the unit-cell scale. We used these capabilities to manipulate and reveal individual oxygen vacancies at 90° domain walls in $BaTiO_3$ single crystallites. Using advanced transmission electron microscopy (TEM) methods, we present the charge and strain distribution around these vacancies, demonstrating the formation of a topological solition, quadrupole, allowing us to show qualitatively and quantitatively the origin of domain-wall charging. Moreover, we demonstrate the stability limits of these pinning sites. Acknowledgment - We thank the support from the Zuckerman STEM Leadership Program, the Technion Russel Barry Nanoscience Institute, Pazy Research Foundation, and the Israel Science Foundation. We also thank Dr. Yaron Kauffman and Mr. Michael Kalina for their technical support.

11:30 AM

(EMA-252-2022) Electrostatically Mediated Polar Topologies and Switching Dynamics in Dielectric-Ferroelectric Nanocomposites

K. Co*[1]; J. Mangeri[3]; P. Alpay[2]; S. Nakhmanson[2]

1. University of Connecticut, Materials Science and Engineering, USA
2. University of Connecticut, Materials Science and Engineering, USA
3. Luxembourg Institute of Science and Technology, Materials Research and Technology, Luxembourg

Interfacial phenomena in dielectric-ferroelectric composite systems hold significant potential for promoting and stabilizing novel properties. In this work we utilize a computational Landau-Ginzburg-Devonshire phenomenological theory-based approach to elucidate the influence of electrostatic self-interaction on the polarization behavior of spherical ferroelectric nanoparticles embedded in a dielectric matrix. By varying the particle volume and the dielectric permittivity of the surrounding medium, phase boundaries between states with polarization patterns exhibiting monodomain, domain-wall, vortex, and paraelectric topologies are observed in isolated particles. Under an applied bias, incomplete screening of surface charges can lead to a size-dependent, monodomain-to-vortex topological phase transition that suppresses macroscopic polarization before the field switches. The vortex topology observed in the polarization-suppressed region of the system P-E dependence minimizes the macroscopic charge on the particle-matrix interface, resulting in the double hysteresis loop shapes that are characteristic for antiferroelectrics. In multiparticle systems, closely packed particle arrays with switching dynamics akin to isolated behavior can be assembled by controlling the polar states topology and the screening strength of the dielectric matrix.

11:45 AM

(EMA-253-2022) 3D structure–property correlations of emerging ferroelectric materials revealed by tomographic atomic force microscopy (Invited)

J. SONG*[1]; S. T. Jaszewski[2]; S. Wang[3]; A. Chen[4]; L. You[3]; J. Ihlefeld[2]; B. Huey[1]

1. University of Connecticut, Materials Science and Engineering, USA
2. University of Virginia, Department of Materials Science and Engineering, USA
3. Soochow University, School of Physical Science and Technology, China
4. Los Alamos National Lab, USA

With the ever-increasing complexity in the structure and design of advanced functional materials, encompassing single crystals and epitaxial heterostructures and superlattices, polycrystallinity, nanocomposites, mesoporosity, and even van der Waals layers, there is a strong demand for imaging and analysis methods with volumetric property mapping capability at the nanoscale. After a brief review of the tomographic atomic force microscopy (T-AFM) approach, results from several emerging ferroelectric materials are presented. These include the 3D complex domain structures in $BiFeO_3$-$CoFe_2O_4$ nanocomposites, textured polycrystalline HfO_2 thin films, and oxide-free 2D van der Waals ferroelectrics. Thickness scaling of their functional properties are also uniquely accessible, including the polarization magnitude and preferential orientations as well as ferroelectric switching. The novel perspective provided by this multi-dimensional imaging approach, providing insight into correlations between local properties and microstructure, strain, interfaces, and thickness dependences, thereby advances the fundamental understanding and informs practical designs for future ferroelectric materials and devices.

Synthesis, Characterization, and Processing

Room: Cypress B

Session Chair: Kevin Co, University of Connecticut

2:00 PM

(EMA-264-2022) Mg^{2+} Diffusion-Induced Structural and Property Evolution in Epitaxial Fe_3O_4 Thin Films (Invited)

Y. Du*[1]

1. PNNL, USA

Epitaxial Fe_3O_4 thin films grown on single crystal MgO(001) present well-defined model systems to study fundamental multivalent ion diffusion and associated phase transition processes. In this work, we show at an atomic scale the Mg^{2+} diffusion pathways, kinetics, and reaction products at the Fe_3O_4/MgO heterostructures under different oxygen partial pressures. Combining microscopic, optical, and spectroscopic techniques, we demonstrate that an oxygen-rich environment promotes facile Mg^{2+} incorporation into the Fe^{2+} sites, leading to the formation of $Mg_{1-x}Fe_{2+x}O_4$ spinel structures. Conversely, annealing in vacuum results in the formation of a thin interfacial rocksalt layer with significantly reduced Mg^{2+} diffusion. The observed changes in transport and optical properties are interpreted in light of the electronic structures determined by X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. Moreover, we show that Ca^{2+} impurities in MgO substrates segregate

to the Fe_3O_4/MgO interfaces and act as a blocking layer to the subsequent Mg/Fe diffusion. Our results reveal the critical role of available anions and cation impurities in governing cation diffusion in the spinel structures and the need to prevent formation of unwanted reaction intermediates for the promotion of facile cation diffusion.

2:30 PM

(EMA-265-2022) Strain tuning of magnetic and optical properties in epitaxial rare earth chromide single crystal thin films

B. Paudel*[1]; Y. Sharma[2]; A. Chen[2]; Y. Du[1]

1. Pacific Northwest National Laboratory, USA
2. Los Alamos National Laboratory, USA

The effect of epitaxial strain on magnetic and optical properties of perovskite LaCrO3 (LCO) single crystal thin films deposited via pulsed laser epitaxy is studied. To impose the compressive and tensile strain states, epitaxial LCO films are deposited with a proper choice of the substrates. A combined experimental and theoretical approach is used to demonstrate the direct correlation between lattice-strain and functional properties. The magnetic measurements show that the lattice anisotropy plays a critical role in controlling the magnetic aniostropy and net magnetic moment of LCO films. The strain induced tetragonal distortion in the film lattice strongly affects the optical transitions and charge transfer gap in LCO. These results indicate that the strain controlled lattice modifications could be key for unveiling novel functional properties of perovskite rare-earth chromites and related material systems.

2:45 PM

(EMA-266-2022) Flexo-phototronic Effect in Centro-symmetric $BiVO_4$ Epitaxial Films (Invited)

P. Shao[1]; Y. Chu*[1]

1. National Chiao Tung University, Materials Science and Engineering, Taiwan

With exciting functionality, topological defects in ferroic system have attracted much attention. Under proper design, the emergence of polar domain walls in non-polar ferroelastics enables flexo-phototronic effect. In this study, we revealed ferroelastic twin texture with localized flexoelectric effect in epitaxial $BiVO_4$ film by piezoresponse force microscopy. Supported by the strain field analysis, we found the piezoresponse confined at domain wall area is attributed to the flexoelectric effect induced by the presence of ferroelastic twin domains during the paraelastic to ferroelastic phase transition. The mechanism of flexo-phototronic was further supported by dye-degradation and generation of reactive radicals experiments. This work not only provides new insights into the introduction of flexo-phototronic effects in non-polar materials, but also sheds light on a new concept to use material inhomogeneity for acquiring multifunctionality.

3:15 PM

(EMA-267-2022) Modeling Thermoelectric Properties of Polycrystalline Materials at Mesoscale

D. Basaula*[1]; M. Daeipour[1]; L. Kuna[2]; J. Mangeri[3]; B. Feygelson[2]; S. Nakhmanson[4]

1. University of Connecticut, USA
2. U.S. Naval Research Laboratory, USA
3. Luxemburg Institute of Science and Technology, Luxembourg
4. University of Connecticut, Materials Science and Engineering, USA

A finite element method-based approach has been developed for evaluating the thermoelectric properties of polycrystalline materials at the mesoscale. This approach was first validated for isotropic systems by simulating effective Seebeck effect in a thermocouple and Peltier cooling at an interface between two dissimilar materials, obtaining good agreement with prior experimental or computational results. The developed approach was then used to model coupled heat and electrical current flow through an anisotropic polycrystalline material, providing local temperature and electric potential distributions under different applied conditions. This computational framework establishes the foundation necessary to elucidate the intricacies of coupled thermal and electric conduction through geometrically complex materials, including polycrystals, nanostructures and nanocomposites, and could provide new insights for improvement of their operational efficiency.

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

Applied Superconductors: Flux Pinning and Critical Currents

Room: Orange B
Session Chair: Michael Sumption, Ohio State University

8:30 AM

(EMA-208-2022) Comparison of current and loss metrics for superconductors, cryo-conductors, and CNT based composites at high frequencies for aircraft propulsion applications, comparison to conventional conductors (Invited)

M. D. Sumption*[1]

1. Ohio State University, MSE, USA

Motors and generators with power densities in the 30-40 kW/kg are of great interest for electric aircraft propulsion. In order to reach these power densities while retaining machine efficiency, high current, low loss advanced conductors are required. Superconductors have very high current densities, but suffer from AC losses at higher frequencies, while conventional approaches are limited by ohmic losses. In this work a comparison of the AC losses of various advanced conductor options are considered in the context of aircraft propulsion motor applications, specifically stators, which are the most demanding in terms of loss control. The influence of Litz cabling (Cu, Al), multifilamentary structure (superconductors and hyperconductors), and conductor anisotropy and fibrosity (CNT Yarns and metallized yarns) are compared. Skin depth effects are discussed for both monolithic and composite structures. Conductor metrics are then discussed. It is shown that there are significant similarities in loss treatment and skin depth regimes for conductors with multifilamentary or fiberous structures whether superconducting or not. Finally, regimes of competitiveness are discussed for various existing and potential conductors, in the context of high power density aircraft propulsion applications.

9:00 AM

(EMA-209-2022) Application of metamaterial nano-engineering for increasing the superconducting critical temperature (Invited)

M. Osofsky*[1]; V. Smolyaninova[2]; J. Prestigiacomo[1]; H. Kim[1]; N. Bassim[3]; I. Smolyaninov[4]

1. Naval Research Laboratory, USA
2. Towson University, USA
3. McMaster University, Materials Science and Engineering, Canada
4. University of Maryland, Electrical and Computer Engineering, USA

We have demonstrated that the metamaterial approach to dielectric response engineering increases the critical temperature of a composite superconductor-dielectric system in the epsilon near zero (ENZ) and hyperbolic regimes. To create such metamaterial superconductors three approaches were implemented. In the first approach, mixtures of tin and barium titanate nanoparticles of varying composition were used. An increase of the critical temperature of the order of 5% compared to bulk tin has been observed for a 40% volume fraction of barium titanate nanoparticles. Similar results were also obtained with compressed mixtures of tin and strontium titanate nanoparticles. In the second approach, we demonstrate the use of Al_2O_3-coated aluminium nanoparticles to form an ENZ core-shell metamaterial superconductor with a T_c that is three times that of pure aluminium.

In the third approach, we demonstrate a similar T_c enhancement in thin Al/Al_2O_3 heterostructures that form a hyperbolic metamaterial superconductor. IR reflectivity measurements confirm the predicted metamaterial modification of the dielectric function thus demonstrating the efficacy of the metamaterial approach to T_c engineering. The developed technology enables efficient nanofabrication of bulk aluminium-based metamaterial superconductors.

9:30 AM

(EMA-210-2022) Search for Advanced Electric Conductors for Aerospace Applications (Invited)

T. J. Haugan*[1]; C. Kovacs[2]

1. U.S. Air Force Research Laboratory, Aerospace Systems Directorate, USA
2. Scintillating Solutions LLC, USA

The generation, distribution and control of electric power is fundamental to every electronic industry, and power levels range from even milliwatts up to 10's of Gigawatts. Essential elements of electric power systems include electric conductors, and for aerospace they are the major weight percentage (surprisingly, by-far) of aircraft electric components and systems. For microelectronic integrated circuits, the heat loss of Cu/Al interconnects has stopped Moore's law of progress, and reduce the system-level switching speed by > 100x. And for Quantum Information Technology (QIT), as systems scale to larger size, the quantum interconnect (QuIC) bottleneck is imminent, and emerging as a grand challenge. The solutions for these technology challenges is similar, to discover/develop electric conductors that have superior electrical conductivity to standard materials, including Cu, Cu-clad Al (CCA), and Al. And for aerospace applications, there is a need to greatly increase the mass-specific electrical conductivity, for which Al is 2x higher than Cu. This talk will introduce and review these topics, and potential materials classes that can be studied to increase the mass-specific electrical conductivity, for wide ranges of temperature needed from 50 mK to > 1000 K. Potential classes of materials to consider include carbon allotropes, delafossites, Weyl metals, and other.

10:30 AM

(EMA-211-2022) Increased Current Density and Pinning Force in Ca-Doped $YBa_2Cu_3O_{7-\delta}$ / $BaZrO_3$ Multilayer Thin Films

M. Sebastian*[1]; V. Ogunjimi[2]; B. Gautam[2]; C. Ebbing[1]; D. Zhang[3]; J. Jian[3]; J. Huang[3]; Y. Zhang[3]; H. Wang[5]; J. Wu[2]; T. J. Haugan[4]

1. University of Dayton Research Institute, USA
2. University of Kansas, USA
3. Purdue University, Materials Engineering, USA
4. Air Force Research Lab, Aerospace Systems Directorate, USA
5. Purdue University, Materials Engineering, USA

An important research goal in the applications of high temperature superconductor $YBa2Cu_3O_{7-\delta}$ (YBCO) thin films is increasing both the critical current density and also the isotropic nature of the film. YBCO is inherently anisotropic due to its layered perovskite structure. The critical current density of YBCO thin films is enhanced by increasing the flux pinning sites in the film by the addition of insulating nano-phase materials, such as $BaZrO_3$ (BZO) nano-rods, which are also anisotropic in nature. Using a multilayer pulsed laser deposition technique has been shown to produce films with inclusions that are more isotropic in nature. However, the defective BZO nanorod interface, resulting from its lattice mismatch with YBCO, prevents obtaining optimum pinning force. This research explores the effect of Ca doped YBCO space layers in the multilayer composite film, on the BZO nanorod / YBCO interface. The interplay of combining these three variables: $BaZrO_3$ addition to YBCO, multilayer film growth resulting from varying pulsed laser deposition conditions, and employing Ca doped YBCO space layers; and the resulting impact on film microstructures and superconducting properties, will be presented.

10:45 AM

(EMA-212-2022) Magnetization Creep of $Y_1Ba_2Cu_3O_{7-x}$ Thin Films with Columnar Y_2BaCuO_5 and $BaZrO_3$ Pinning Centers Additions (Invited)

C. Myers*[1]; M. A. Susner[2]; M. Sebastian[3]; D. Zhang[6]; J. Wu[5]; H. Wang[7]; M. D. Sumption[8]; T. J. Haugan[4]

1. Lawrence Berkeley National Laboratory, ATAP/BCMT, USA
2. The Air Force Research Laboratory, USA
3. UDRI, USA
4. U.S. Air Force Research Laboratory, Aerospace Systems Directorate, USA
5. University of Kansas, USA
6. Purdue University, Materials Engineering, USA
7. Purdue University, School of Materials Engineeringn, USA
8. Ohio State University, MSE, USA

YBCO coated conductors are being considered for use in high-field magnets for future particle accelerators, but they possess large effective filament diameters, which could degrade the field quality of a magnet built from them. Techniques exist to reduce the field errors resulting from these static magnetic moments, but coated conductors also exhibit flux creep, even at 4 K. This creep reduces the magnetic moment with time, which may necessitate complicated active correction to rectify the subsequently changing field error. Secondary phases can be introduced to the YBCO matrix to alter the critical current of the superconductor by pinning the flux. Here we study the magnetization and flux creep in two sets of YBCO films. One set was made using pulsed laser deposition and included samples with 0, 5, and 10 vol.% Y211, and one sample containing 2 vol.% BZO. A second set was made using chemical vapor deposition and included 0, 7.5, and 25 mol.% BZO. The 4 K M-H and magnetic relaxation of the samples from 4-70 K and in fields from 1-8 T was measured. The data of these experiments were analyzed using Collective Pinning theory to extract intrinsic pinning potentials (U_0) and rank the samples based on pinning strength. The nanostructure and morphology of the samples was studied using transmission electron microscopy and the results were compared to the magnetic analysis.

S8: Structure–Property Relationships in Relaxor Ceramics

Advanced nano- and Microscale Characterization Methods for Relaxors

Room: Cypress C
Session Chairs: Abhijit Pramanick, City University of Hong Kong; Stephen Funni, North Carolina State University

8:30 AM

(EMA-213-2022) Direct Imaging of Fractal-Dimensional Percolation in the 3D Cluster Dynamics of a Perovskite Supercrystal (Invited)

L. Falsi*[1]; M. Aversa[1]; F. Di Mei[1]; D. Pierangeli[1]; F. Xin[1]; A. Agranat[2]; E. DelRe[1]

1. University of Rome "La Sapienza", Department of Physics, Italy
2. Hebrew University, The Brojde Center for Innovative Engineering and Computer Science, Israel

To date, no direct volume imaging technique is available to investigate transition dynamics in transparent bulk ferroelectrics. The problem is that each single cluster can form in a volume with a size that can range from tens to hundreds of nanometers and this makes direct wide-area imaging generally unfeasible. We use giant optical refraction to perform, for the first time, real-time imaging of ferroelectric volume cluster dynamics. Experiments are carried out in biased nanodisordered bulk KTN:Li perovskite kept below its room-temperature Curie point. The analysis of polarization transmission images through the sample versus electric field indicates two

distinct percolative transitions at two electric field thresholds. The low-field transition involves a directional fractal chain of dimension D=1.65, while the high-field transition has a dimension D>2, as the sample undergoes a transition from a highly organized supercrystal state to a disordered ferroelectric cluster state. Phenomenology is interpreted in terms of biased vortex geometries in a full 3D mosaic and forms further evidence of the role played by 3D vortices in the mesoscopic physics of solid-solution ferroelectric cooled below their Curie point. The direct observation, in the transparent volume, of percolating cluster dynamics sheds light on the nature and susceptibility of ferroelectric supercrystals.

9:00 AM

(EMA-214-2022) Maximum Entropy Method for Identifying Disordered Displacements in Relaxors (Invited)

W. Surta*[1]; M. Rosseinsky[1]; J. Claridge[1]; A. J. Bell[2]

1. University of Liverpool, Chemistry, United Kingdom
2. University of Leeds, Instituute for Materials Research, United Kingdom

Relaxors present a great challenge in electroceramics as their physical response is very attractive, but the origin this response expresses itself on a length-scale which is challenging to probe. Standard techniques such as XRD lose their utility as diffraction patterns often reveal a cubic structure, precluding the observed properties. These difficulties result in "pseudocubic" structural descriptions with little additional detail, but understanding the nature of the disordered cation displacements in relaxors is vital to tailoring the physical response. Despite appearing information poor, there are methods which can utilize these diffraction data in a robust way. One such tool is the maximum entropy method, an ab initio method that uses the observed structure factor from a diffraction pattern. This method has found utility in ferroelectric research for many years allowing the visualization and quantification of bonding interactions. Its recent adaptation for use with relaxors has proved that it is a useful tool for identifying local displacements masked within large atomic displacement parameters. This method represents a powerful new tool for researching relaxors and holds potential for the detailed extraction of important structural information from cubic diffraction patterns, key to understanding the short range ordering and resultant physical properties in relaxor based electroceramics.

9:30 AM

(EMA-215-2022) Processing-related microstructural features mediating the enhancement of ferroelectric and electrocaloric properties in relaxor ceramics (Invited)

B. Rozic*[1]; H. Uršič[2]; L. Fulanovic[3]; A. Bradesko[2]; T. Rojac[2]; V. Bobnar[1]; B. Malic[2]; Z. Kutnjak[4]

1. Jozef Stefan Institute, Department of Condensed Matter Physics, Slovenia
2. Jozef Stefan Institute, Electronic Ceramics Department, Slovenia
3. TU Darmstadt, Nonmetallic- Inorganic Materials, Germany
4. Jozef Stefan Institute, Slovenia

The impact of synthesis-mediated microstructural features such as grain size and shape on ferroelectric, piezoelectric, electrocaloric properties are reviewed. It is shown that a substantial enhancement of the electrocaloric effect can be achieved with a properly engineered ceramic microstructure in PMN-xPT relaxors. It is shown by dielectric, PFM, and direct electrocaloric measurements that growth rate controlled stoichiometry of fiber crystals could result in optimized lead-free BCZT crystals with enhanced energy storage, piezoelectric and electrocaloric properties. We demonstrate that the microstructural features such as increased ceramics' grain boundary conductance caused by an electric-field-induced phase transformation to a ferroelectric phase are directly responsible for the electrocaloric fatigue. The method how to avoid such fatigue is also discussed.

Local Structure of Relaxors

Room: Cypress C

Session Chairs: Wesley Surta, University of Liverpool; Ilya Grinberg, Bar Ilan University

10:30 AM

(EMA-254-2022) Characterization of local atomic structure of relaxors for energy applications using quantum beams (Invited)

A. Pramanick*[1]

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

Relaxors are promising materials for energy-related technologies, such as high-power energy storage, pyroelectric energy harvesting, and electrocaloric cooling. For the rational design of relaxors for energy applications, clear elucidation of their structure-property relationships is a prerequisite. Nevertheless, relaxors are challenging to understand from a structural viewpoint. Although large functional properties of relaxors are conventionally attributed to the presence of nanoscale domains called polar nanoregions (PNR), the spatial/temporal correlations of local dipoles within the PNRs are highly debated. Recent studies with more powerful characterization tools have further emphasized the complexity of local atomic structure in both traditional Pb-based and new environmentally friendly Pb-free relaxors. In this talk, I will present our recent findings on the local polar atomic displacements in Pb-free relaxor ceramics, which are characterized by pair distribution function analysis of x-ray/neutron total scattering patterns. I will also demonstrate the application of the dynamic pair distribution function (DyPDF) method to elucidate the dynamic fluctuations of short-range atomic correlations within PNRs over THz timescale. Correlations between local atomic structure and dynamics in relaxors and their functional properties for energy-related applications will be discussed.

11:00 AM

(EMA-255-2022) Quantifying local structural correlations in relaxor and classical ferroelectrics through STEM (Invited)

S. Funni*[1]; S. Calderon[1]; E. Dickey[1]

1. Carnegie Mellon University, Materials Science and Engineering, USA

Local chemical and structural deviations govern the properties of many functional materials, including relaxor ferroelectrics. X-ray and neutron scattering have historically played leading roles in understanding local structure and remain important characterization techniques. More recently, aberration-corrected scanning transmission electron microscopy (STEM) has provided unique insights into local structure and chemistry via real-space imaging at atomic resolution. From various STEM modalities, the cation and anion sublattices of complex oxides can be imaged at atomic scale. Such data provides projected unit-cell mapping of local structure, strain and polarization. To statistically represent the local structure and to extend the analysis to medium and long-range order, we have recently developed the vector pair correlation function (vPCF), which is directly calculated from STEM lattice images. We will present examples of vPCF analysis of complex ferroelectric, including perovskite and tungsten bronze systems, and demonstrate the ability to quantify local structure and ordering on a sublattice specific basis while identifying correlation lengths of various phenomena. 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.

11:30 AM

(EMA-256-2022) Soft mode and low-frequency lattice dynamics from $BaZrO_3$ single crystals

C. Toulouse[1]; C. Milesi-Brault[2]; F. Bourdarot[4]; A. Piovano[4]; A. Bossak[3]; M. Guennou*[1]

1. University of Luxembourg, Luxembourg
2. Luxembourg Institute of Science and Technology, Luxembourg
3. European Synchrotron Radiation Facility, France
4. Institut Laue Langevin, France

Barium zirconate $BaZrO_3$ is one of the end-member of the lead-free relaxor BZT, and itself a simple perovskite that experimentally remains cubic down to the lowest temperatures. However, it has been known for a long time that standard first-principle calculations predict the cubic structure to be dynamically unstable, with an unstable soft phonon mode corresponding to tilts of the oxygen octahedra, which is beleived to play a role in its physical properties. Experimentally, direct lattice dynamical studies have been limited by the scarcity of single crystals, themselves due to the very high melting point of $BaZrO_3$. As a result, most studies have been restricted to polycrystalline materials, and have allowed for indirect estimations only of the real frequency of the unstable tilt mode. Here, we take advantage of our previous growths of $BaZrO_3$ single crystals to investigate directly the low-frequency lattice dynamics across the Brillouin zone. Crystals grown by the floating zone technique in particular were found to be large in size and suitable for inelastic neutron scattering. Together with complementary studies by inelastic X-ray scattering, we could successfully measure the soft tilt mode at 8 meV at room temperature and unveil its strong softening down to low temperatures. The relation with physical properties will be described.

Applications of Relaxors

Room: Cypress C

Session Chairs: Ludovica Falsi, University of Rome, "La Sapienza"; Valentino Cooper, Oak Ridge National Laboratory

11:45 AM

(EMA-257-2022) Lead-free electroceramics for high energy-density multilayer ceramic capacitors (Invited)

G. Wang*[1]; D. C. Sinclair[1]; I. M. Reaney[1]; Z. Lu[1]; d. wang[2]

1. University of Sheffield, Materials Science & Engineering, United Kingdom
2. Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China

Materials exhibiting high energy/power density are currently needed to meet the growing demand of portable electronics, electric vehicles and large-scale energy storage devices. Compared to fuel cells, batteries, and supercapacitors, conventional dielectric capacitors are receiving increased attention for pulse power and power electronic applications due to their high energy density and their fast charge-discharge speed. The key to high energy density in dielectric capacitors is a large Δpolarisation (maximum-remanent) and a high electric breakdown strength. Lead-free bulk electroceramics, i.e. $BiFeO_3$-based, $Na_{0.5}Bi_{0.5}TiO_3$-based and $BaTiO_3$-based, have been reported with superior energy density and simultaneously can be transferred into excellent multilayer ceramic capacitors. My talk would like to firstly provide a comprehensive review of the state-of-the-art, followed by a discussion on few of key factors (with examples) to improve energy storage properties, such as control of local structure, conductivity and electrical homogeneity.

12:15 PM

(EMA-258-2022) Non-ergodic to ergodic relaxor evolution in some Pb-free perovskites

A. Feteira*[1]

1. Sheffield Hallam University, United Kingdom

In this study it is shown that minor levels ceramics leads to transition from non-ergodic to an ergodic relaxor behaviour in BNT-BT and BKT-BNT-BT. With certain dopants this is accompanied by the emergence of giant field-induced strains, however those show high temperature dependences and also large hysteresis, precluding their application as piezo actuators. At lower applied fields, respectable electric-field induced strains are achievable, which show a much better temperature stability and less hysteresis.

Multiscale Modelling and Computational Materials Design of Relaxors

Room: Cypress C

Session Chairs: Antonio Feteira, Sheffield Hallam University; Brigita Rozic, Jozef Stefan Institute

2:00 PM

(EMA-268-2022) Computational design strategy for disordered complex oxides (Invited)

V. R. Cooper*[1]

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA

High entropy, multi-component metal alloys, have superior mechanical properties and high radiation tolerances; which are, in part, driven by configurational entropy. Recently, an oxide analogue comprised of MgO, CoO, NiO, CuO and ZnO was synthesized; exhibiting a truly entropy-stabilized, reversible phase transition from a multiphase material to a single rock salt-ordered phase above 850-900°C. This entropy-driven stabilization may engender many unique properties, such as high melting temperatures, radiation resistance and other anomalous responses. Here, we discuss a design strategy for the prediction of synthesizable disordered oxides. Our effort employs first principles studies of 2-component oxides to develop design rules based on the relationship between pairwise enthalpies of formation, ΔH, and configurational entropy of the disordered material. A similar chemical identity-to-ΔH map was previously explored using the class of high entropy alloys, where the stability of multicomponent metal alloys was correlated to the enthalpy of mixing of binary and ternary compounds. Here, the focus will be on the exploration and discovery of synthesizable entropy-stabilized compounds with novel functionalities. This work was supported by the U.S. D.O.E., Office of Science, BES, MSED using resources at NERSC and OLCF.

2:30 PM

(EMA-269-2022) Understanding how composition controls properties in relaxor ferroelectrics (Invited)

I. Grinberg*[1]

1. Bar Ilan University, Chemistry, Israel

Relaxor ferroelectrics have been investigated for over six decades due to their fascinating physical behavior and excellent properties that enable high-performance technological applications. Recent advances in computational power and techniques have enabled multiscale studies that have significantly enhanced the understanding of the physics of relaxors and in particular the relationship between their composition, structure and properties. Such understanding is vital for rational design of new materials. In this talk, I will review the current understanding of relaxor structure and physics and will discuss our latest results on how the changes in the solid solution composition change relaxor structure and properties

such as dielectric dispersion, transition temperature, coercive field and piezoelectric coefficient as revealed by DFT and MD simulations and analytical modeling.

S9: Ion-conducting Ceramics

Ionic-conducting Ceramics for Energy Storage / Synthesis and Processing Conditions on Ionic Conduction

Room: Magnolia A
Session Chair: Hua Zhou, Argonne National Lab

8:30 AM

(EMA-216-2022) Electrochemical properties of $Sr_3Fe_{1.8}Co_{0.2}O_7$ as solid oxide fuel cell cathode

A. nemati*[1]; A. Ghani Harzand[2]; M. Golmohammad[3]; A. Malek Khachatourian[2]

1. Sharif University of Technology, Tehran, Iran, Materials Science & Eng., Islamic Republic of Iran
2. Sharif University of Technology, Materials Science & Eng., Islamic Republic of Iran
3. Niroo Research Institute (NRI), Renewable Energy Department, Islamic Republic of Iran

In the solid oxide fuel cells (SOFCs) the high temperature is the main shortcoming for commercialization. To achieve intermediate temperature SOFCs one needs to have the conductivity of cathode materials at lower temperatures. In this study, a conductive $Sr_3Fe_{1.8}Co_{0.2}O_7$ cathode material with the Ruddlesden–Popper crystal structure was synthesized. The effect of sintering temperature was investigated. To evaluate the sintering effect on the electrochemical behavior of the powder, a paste of powder was painted on both sides of the Gadolinium doped Ceria electrolyte and sintered at 1000°C and 1100°C. Besides, the electrical conductivity of the sample was determined by the four-point probe electrical conductivity method in the temperature range 200-800°C in the atmosphere. XRD and FESEM were used to characterize the samples. FESEM micrographs showed that the particles are rod-shaped with an average particle size of 670 nm. The electrochemical impedance analysis on symmetrical half-cells revealed that the minimum polarization resistance for the sintered cathode at 1000°C and 1100°C was determined 1.1 Ohms-cm^2 and 1.6 Ohms-cm^2 at 800 °C, respectively. It was observed in the FESEM micrograph that transport pathways for oxygen ions conduction were decreased at higher sintering temperatures. The obtained results showed that the maximum electrical conductivity at 427°C was 76 S.cm^{-1}.

8:45 AM

(EMA-217-2022) Controlling Defect Fluorites via Oxidative Charge Ordering in $Sc_2V_{1-x}Ti_xO_{5+\delta}$

B. N. Richtik*[1]; D. Vrublevskiy[2]; C. Wiebe[3]; M. Bieringer[2]

1. University of Calgary, Chemistry, Canada
2. University of Manitoba, Chemistry, Canada
3. University of Winnipeg, Chemistry, Canada

The defect fluorite is currently the most common electrolyte used in solid oxide fuel cells. The disordered anionic lattice, with respect to oxide ions and vacancies, within the defect fluorite allows for ion conduction. Hence maintaining disorder during synthesis and use is key to sustain a functional electrolyte. This work is focused on understanding the relationship between order and disorder within defect fluorite structures and how to avoid forming ordered phases that would prevent ion conduction. Here we investigate a series of $Sc_2V_{1-x}Ti_xO_{5+\delta}$ phases that can crystallize in the bixbyite, defect fluorite, tetragonal-Sc_2VO_5, or pseudobrookite structures. Structures were prepared via conventional solid state synthesis and a detailed structural analysis was conducted including x-ray and neutron diffraction, XANES and DC magnetic susceptibility measurements. We demonstrate that order/disorder within these phases can be altered by varying the charge and size of cations, and the oxygen stoichiometry. We show that the oxidation state of vanadium can be controlled which allows us to navigate between these structures through control of redox chemistry.

9:00 AM

(EMA-223-2022) In Situ Spatially-Resolved Thermal Conductivity Mapping of Battery Cell Degradation

M. Milich*[1]; Z. Nie[2]; G. Koenig[2]; J. Tomko[1]; P. E. Hopkins[1]

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

One of the primary challenges in limiting improvements in energy storage technologies is degradation and thermo-mechanical failure of localized regions after many on/off cycles. For example, as battery cells are subjected to large numbers of charge/discharge cycles, damage is found to be highly localized to regions corresponding to the largest temperature rises. These "hot spots" tend to have a reduced thermal conductivity and, in turn, induce even larger temperature rises and further damage within the cell. Device degradation yields an increased resistance to ion transport between anode and cathode, lowering the charge capacity of the cell while increasing the time required to charge it. By spatially mapping the thermal conductivity of a battery cell over the course of a charge and discharge cycle, we are able to capture the formation and evolution of these hot spots, and characterize their effects on local heat dissipation. For this study, steady-state thermoreflectance (SSTR), an optical pump-probe technique, is used to measure the spatially varying thermal conductivity of the anode of a lithium-ion battery cell at 0%, 20%, 50%, and 100% of full charge capacity, as well as after complete discharge. Based on these maps, we identify areas of damage formation and quantify the resulting local changes in thermal diffusivity.

9:15 AM

(EMA-218-2022) Effects of Li Vapor Overpressure on the Microstructure, Composition, and Ion Conductivity of Perovskite $Li_{3x}La_{1/3-x}TaO_3$ Ion Conductors

I. A. Brummel*[1]; H. J. Brown-Shaklee[2]; K. Wynne[3]; W. A. Lanford[3]; J. Ihlefeld[4]

1. University of Virginia, Materials Scienc and Engineering, USA
2. Sandia National Laboratories, USA
3. State University of New York at Albany, Department of Physics, USA
4. University of Virginia, Department of Materials Science and Engineering, USA

A combustion synthesis methodology for the preparation of perovskite $Li_{3x}La_{1/3-x}TaO_3$ lithium-ion conductors with x=0.033 is presented. Bulk ceramic specimens were prepared under different lithium vapor overpressure conditions governed by combinations of burial powder and cover crucibles. Specimens were batched with a nominal lithium excess of 20 at%, to account for losses during sintering. All specimens were observed to exhibit tetragonal symmetry as a result of La ordering along the c-axis. The lithium content was determined using nuclear reaction analysis with the $^7Li(p,\alpha)^4He$ reaction. Room temperature lithium-ion conductivity varied depending upon lithium over-pressure during sintering and a maximum of 6.0×10^{-6} S/cm was observed for pellets sintered with a cover crucible sealed with parent powder. Both the inter- and intra-granular ion conductivities were maximized under the same condition. Schottky barrier effects at grain boundaries were explored by impedance spectroscopy using differing DC biases. The ion conductivity was found to be independent of applied DC bias, implying grain boundary conductivity effects are not governed by Schottky barriers. Grain sizes determined from backscatter SEM micrographs showed no correlation to the observed trend in ion conductivity.

9:30 AM

(EMA-219-2022) Structure-property relationship of garnet type $Li_5La_3(Nb_xTa_{1-x})_2O_{12}$ solid-state solution as a function of sintering temperature.

A. P. Kafle*[1]; W. Wong_Ng[2]; B. Dutta[3]; G. R. Stafford[2]; V. P. Oleshko[2]; I. Pegg[1]; J. Kaduk[4]

1. The Catholic University of America, Physics, USA
2. National Institute of Standards and Technology, USA
3. Catholic University of America, Physics, USA
4. Northern Central College, Chemistry, USA

Garnet type ceramic solid solutions of the lanthanide series, $Li_5R_3M_2O_{12}$, have been explored for their potential applications in all solid-state batteries as high ionic conductivity electrolytes. In this work, a series of compounds based on the nominal composition $Li_5La_3(Nb_xTa_{1-x})_2O_{12}$ (x = 0.1 to 0.9), was prepared using the conventional solid state reaction technique. These $Li_5La_3(Nb_xTa_{1-x})_2O_{12}$ phases were found to be cubic, with the space group Ia-3d. One member of the solid solution was selected for a further detailed study. Sample characterization was carried out using XRD, FESEM-EDX, and S/TEM-EDX-EELS. The Li-ion conductivity was measured by an AC impedance spectrometer with a custom-modified attachment for sample handling. This paper discusses the structure-property relationship as a function of sintering temperature.

9:45 AM

(EMA-220-2022) Cold Sintering of Solid-State Sodium-ion Battery Composites which address Co-sintering and Mixed Conduction Issues

Z. Grady*[2]; A. Ndayishimiye[1]; Z. Fan[1]; C. Randall[2]

1. Materials Research Institute, USA
2. Penn State University, Materials Science and Engineering, USA

Solid-state batteries, while a promising technology, remain plagued by numerous outstanding technical problems. One of the most glaring is the thermal gap between the solid-state electrolyte (SSE) sintering temperature and the window of thermal stability for other electrode materials (e.g., active materials, carbon). This prevents the facile fabrication of co-sintered layered structures containing arbitrary compositions with mixed ionic and electronic conductivity. Cold sintering is a nascent sintering technique that lowers the sintering temperature from the conventional T_{sinter} > 1200°C to under 400°C. It is hypothesized that cold sintering might enable the fabrication of unprecedented electrode microstructures containing electron and ion conductors, which can then co-sintered in a layered structure with SSEs. To illustrate this, this talk specifically discusses the effectiveness of cold sintering on SSE chemistries ranging from NASICON to β''-Al_2O_3. The SSEs are then combined with active materials and carbon to demonstrate the tunability of the mixed conducting properties. Finally, these materials are evaluated electrochemically, and future opportunities and challenges are discussed.

10:30 AM

(EMA-221-2022) Ultrafast high-temperature sintering of $Li_7La_3Zr_2O_{12}$ solid electrolyte

M. Ihrig*[1]; W. Rheinheimer[1]; M. Finsterbusch[1]; O. Guillon[1]

1. Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research, Materials Synthesis and Processing (IEK-1), Germany

All-solid-state Li batteries are regarded as the systems of choice for future mobile electrochemical energy storage. One of the most promising ceramic electrolytes due to its high ionic conductivity and stability against Li metal is the garnet-based Li7La3Zr2O12 (LLZ). While the properties of LLZ are promising, its integration into all-solid-state Li batteries is hampered due to the required high temperature and long times for sintering that decomposes the cathode materials. Advanced sintering techniques, such as ultrafast high-temperature sintering, have shown to significantly increase the sintering rate. Direct contact to graphite heaters allows sintering within seconds due to extremely high heating rates and temperatures. Although the sintering time is only 10 seconds, the density and mechanical stability of the sintered LLZ is promising. The microstructure shows well-formed percolation pathways leading to a high total Li-ion conduction, comparable with conventional sintered LLZ. A high phase purity is reached in vacuum and Ar atmosphere. When using Ar atmosphere, a higher phase purity can be obtained, which is beneficial for the ionic conductivity.

10:45 AM

(EMA-222-2022) Effect of oxygen vacancy on Li-ion diffusion in the Perovskite-Type Solid Electrolyte

J. Hwang*[1]; J. Lee[1]; H. Ju[2]; E. Park[2]; Y. Kim[2]; J. Jang[3]; J. Shim[4]; Y. Kim[2]

1. Pusan National University, Physics, Republic of Korea
2. Sungkyunkwan University, Republic of Korea
3. Korea Basic Science Institute (KBSI), Republic of Korea
4. Dongshin University, Republic of Korea

Solid electrolytes with a fast ion conduction are crucial for all solid batteries. The perovskite-type lithium lanthanum titanate (LLTO) solid electrolytes have been known as one of promising next-generation lithium-ion batteries because they provide high-energy density and superior cyclic stability. However, in spite of these advantages, their practical application is plagued by low ionic conductivity at room temperature. Here, using the first-principles density functional theory calculations, we report that the oxygen vacancies significantly expand the crystal lattice of LLTO solid electrolyte normal to the lithium migration path, resulting in two order of magnitude enhancement in ionic conductivity. Relevant structure reconstructions and underlying mechanism will be discussed in detail at the atomic scale.

11:00 AM

(EMA-224-2022) Structure-Property Relationships of Calcium Tin Gallate Garnets

B. Zanca*[1]; M. Dolgos[2]

1. University of Calgary, Chemistry, Canada
2. University of Calgary, Canada

The discovery of new materials that display oxide ion conductivity is essential for the implementation of solid oxide fuel cell (SOFC) technology. The application range of current materials leads to several mechanical and chemical incompatibility issues between the solid electrolyte and electrode materials leading to device failure. This search for oxide ion conductors has led to the discovery of new garnet materials ($Ca_{2.65+x+y}Sn_{2.65+x-y}Ga_{2.7-2x}O_{12-y}$) which display high temperature conductivity with an oxide ion conduction signature. These materials crystallize in space group (Ia3d), which is typical of most garnets. The Sn4+ occupies all three crystallographic locations in these structures which is noteworthy due to tin siting on both a dodecahedral and a tetrahedral site in an oxide material. The conductivity can be controlled by changing the ratio of cations to decrease the gallium content or to induce oxygen vacancies in the structure resulting in an increase in conductivity by several orders of magnitude. The activation energies were found to be ~0.4 eV between 300–600 °C and ~1.4 eV between 600–800 °C.

S12: 5G Materials and Applications Telecommunications

Measurements

Room: Citrus A
Session Chairs: Florian Bergmann; Geoff Brennecka, Colorado School of Mines

8:30 AM

(EMA-225-2022) Introduction to the Session 12: Materials and Applications in Telecommunications

N. Orloff*[1]

1. NIST, Communications Technology Laboratory, USA

In this talk, I will introduce the session and discuss some emerging trends in telecommunications. I will start by describing what is 5G, millimeter-waves, and the new 6G standards. After reviewing the various technologies and applications, I will talk about how materials research can fill gaps in the literature and our understanding. These gaps will lead us to an overview of the session, cohesively describing how each of the talks might fit into a bigger picture. Join us for 2022's S12: Materials and applications for Telecommunications.

8:45 AM

(EMA-226-2022) Simulation-based resonant imaging of electronic materials for enhanced design in 5G and other emerging technologies (Invited)

M. Celuch*[1]; M. Olszewska-Placha[1]; J. Rudnicki[1]

1. QWED Sp. z o.o., Poland

Resonant methods of electronic material measurements are acknowledged for their supreme accuracy (e.g. for SPDR <0.3% in Dk) and in many cases, the ease of use and relatively low cost, making them affordable to even small labs pursuing the development of novel materials or new applications. The background theory and the state-of-the art in material characterisation with GHz resonators has been presented in our talks at 2020 and 2021 EMA Conferences, and for a more systematic review the reader is referred to a recent paper. In this year's talk, we shall concentrate on recent advances achieved in our own and collaborating laboratories. Our aim is to extend the scope of applications of GHz resonators to higher frequencies (from ca. 1-20 GHz up to 110 GHz), surface imaging (for the detection of defects or surface inhomogeneities), and to new types of energy materials (including battery anodes in H2020 NanoBat project). In all these works, the use of full-wave 3D electromagnetic simulator (QuickWave™ by QWED) has been crucial for both conceptual development and accurate conversion of measured S parameters into materials parameters, of which representative illustrations will be given.

9:15 AM

(EMA-227-2022) Optical arbitrary waveform generation for 5G millimeter-wave measurement (Invited)

B. T. Bosworth*[1]; N. Jungwirth[1]; K. Smith[1]; J. Cheron[1]; F. Quinlan[1]; M. Woodson[2]; J. Morgan[4]; A. Beling[4]; A. Feldman[1]; D. Williams[1]; N. Orloff[3]; C. Long[1]

1. NIST, USA
2. Freedom Photonics, USA
3. NIST, Communications Technology Laboratory, USA
4. University of Virginia, USA

5G millimeter-wave integrated circuits present new challenges for characterization to optimize energy efficiency and performance. Traditional arbitrary waveform generation and nonlinear microwave measurement struggle to cover all the millimeter-wave bands becoming available for 5G wireless communications. Optically derived sources are a potential path to generate arbitrary waveforms up to terahertz frequencies with extremely low noise. In this work, we demonstrate optically derived continuous wave signals with fine phase and amplitude control at (24.8, 49.6, 74.4, 99.2) GHz, within or near new 5G bands. Our approach begins with a 1550 nm electro-optic frequency comb that provides synchronized optical tones across more than a terahertz of bandwidth. A programmable spectral filter applies optical amplitude and phase shifts to individual tones from the optical frequency comb. An on-wafer photodiode then converts this optical signal to large amplitude millimeter-waves with phase and amplitude control. In this way, we demonstrate electronic phase control in 25 milliradian steps and electronic amplitude control in 0.1 dB steps and then apply this control to additive waveform synthesis. We demonstrate optically derived arbitrary repetitive waveform synthesis with 24.8 GHz repetition rate and up to 100 GHz of instantaneous bandwidth.

9:45 AM

(EMA-228-2022) Developing a Standard Reference Material for 5G millimeter wave

L. Enright*[2]; G. L. Brennecka[1]; N. Orloff[2]

1. Colorado School of Mines, USA
2. NIST, Communications Technology Laboratory, USA

In 2019, the National Institute of Standards and Technology discontinued the standard reference material for dielectric constant and loss tangent. Today, there is no standard reference material for those properties. With the development and rollout of 5G millimeter-wave (mmWave) technology, manufacturers need standards to validate measurements techniques, accept new materials, and for quality assurance. While new cavity perturbation fixtures for dielectric measurements are now commercially available for low-loss dielectric measurements, industry still needs a standard to compare the different measurement techniques. Here, we take the first steps to developing a standard reference materials for dielectric constant and loss tangent. We present results from an industry-government round robin used to inform the design of the next standard reference material for dielectric constant and loss tangent. We describe our plans for a new standard and welcome any discussion about how to make these measurements more accessible to the broader community.

10:30 AM

(EMA-229-2022) Innovative Approaches to Solve Low loss Materials Characterization Challenges (Invited)

U. Ray*[1]

1. iNEMI, USA

iNEMI (International Electronics Manufacturing Initiative) has gathered a group of technical experts from 26 companies across the world to address one of the key problems facing the 5G communications world: reliable and reproducible methods of low loss materials characterization to ensure fast product development, avoiding costly learning cycles. The proect involved a collaborative effort of performing round robin measurements across four resonator techniques (SPDR, SCR, BCDR, FPOR) using two reference materials used in the industry (PTFE and COP). The participants included ten laboratories across the globe, in addition to one laboratory that acted as the baseline measurement lab. The results will be presented here, with specific recommendations and call for action for the critical next steps in the 5G/6G arena.

11:00 AM

(EMA-230-2022) Differential measurement techniques for out-of-plane permittivity extraction (Invited)

M. C. Papac*[1]; N. Orloff[1]

1. NIST, Communications Technology Laboratory, USA

The dimensions of conventional microelectronics tend to decrease as telecommunications push to higher frequencies. At millimeter waves, many devices are so small that fabrication tolerances and uncertainties in materials properties can lead to large variability

in device performance. Uncertainty is especially influential on the performance of metal-insulator-metal capacitors. Today, in-plane thin-film permittivity measurements are almost routine. In contrast, out-of-plane permittivity measurement techniques are far less developed, which may be due to the extreme impedance of metal-insulator-metal capacitors, substantial parasitic impedances at high frequency, and the absence of on-wafer calibrations that employ the same electrode configuration as the devices. Here, we discuss our research to quantify the influence of calibration uncertainty on out-of-plane permittivity extraction. As a test case, we explore differential measurement techniques to measure extreme impedances and our plan to maximize measurement sensitivity.

11:30 AM

(EMA-231-2022) Beyond 5G Out-Of-Plane Component of Permittivity Materials Characterization with Latest Commercially Available Solution (Invited)

S. Phommakesone*[1]; D. Kato[1]

1. Keysight Technologies, USA

There are increasing needs to characterize out-of-plane component of permittivity in the past couple of years as more research works are moving up in the frequency range of mmWave and Sub-Terahertz. The in-plane component of permittivity only is not enough as materials are used in more complex device/component design. The most common "Go-To" techniques are Split Post Dielectric Resonators, Split Cylinder Resonators (SPDR), Balanced-type Circular Disk Resonator (BCDR), and Fabry Perot Open Resonator (FPOR), which are shared common features, a general use, and basic theory. Others available techniques are Coplanar Waveguide (CPW), On-Chip Resonator, and Strip-Line, Bereskin or other Transmission Line method. However, only BCDR is suitable for out-of-plane component of permittivity characterization and suitable for very high frequency measurement. With Keysight's BCDR combines with proven performance of mmWave/Sub-THz instruments solves the out-of-plane component of permittivity materials characterization at ease. This module will provide the overall of how BCDR works, measurement tips and sample preparation consideration and more.

12:00 PM

(EMA-232-2022) Industry Panel: Measurements, simulations, and how to do them (Invited)

N. Orloff*[1]

1. NIST, Communications Technology Laboratory, USA

In this panel, we will discuss measurements, simulations, and how to do them. While it may be impossible to exhaustively answer each question, panelists will do their best to identify resources and a discuss different solutions. In addition to discussing measurements, we will also field questions about different electromagnetic simulation techniques and the various software solutions. Attendees can submit during the panel or ahead of time by emailing the session chair. Each question will be read to the panelists and answered during the session. This session is for anyone wishing to learn more about materials measurement and simulations.

Materials

Room: Citrus A

Session Chairs: Meagan Papac, National Institute of Standards and Technology (NIST); Lucas Enright, National Institute of Standards and Technology

2:00 PM

(EMA-270-2022) Broadband permittivity of fused silica glass to 220 GHz

N. Orloff*[1]

1. NIST, Communications Technology Laboratory, USA

Fused silica glass has many excellent electrical, thermal, and mechanical properties. Compared to silicon, it has a relatively low dielectric constant (which permits larger feature sizes) and a very low loss tangent (which improves power consumption). These properties make glass an attractive alternative to composite high density interconnect boards especially for millimeter wave telecommunications. However, high density interconnects boards require thin layers of dielectrics stacked one on top of the other to route electrical signals to different surface mounted packaged components. These thin layers can be as few as 10 micrometers thick or as much as 100 micrometers thick but must be thin to maintain an applications formfactor and thermal handling. Here, we show preliminary results on 100 micrometer thick fused silica that was fabricated using a novel handle wafer process. We show on-wafer permittivity and distributed circuit parameters to 220 GHz, which is well beyond current 5G bands and even covers some new 6G bands. We then compare our on-wafer measurements with split cylinder cavity perturbation techniques up to 80 GHz. As a result, we hope that these measurements might show how thin fused silica glass can impact high density interconnect boards.

2:15 PM

(EMA-271-2022) High Sc-Content (x>0.30) $Al_{1-x}Sc_xN$ Lamb Wave Piezoelectric RF Resonators (Invited)

G. Esteves*[1]; S. Yen[1]; T. Young[1]; Z. Tang[2]; E. Schmidt[1]; L. Gastian[1]; M. D. Henry[1]; T. Bauer[1]; C. Nordquist[1]; R. Olsson[2]

1. Sandia National Laboratories, USA
2. University of Pennsylvania, Department of Electrical and Systems Engineering, USA

Aluminum scandium nitride ($Al_{1-x}Sc_xN$/AlScN) film quality has improved sufficiently to enable the fabrication of RF resonators over the composition range in which the film is piezoelectric (x=0-0.44). However, the addition of Sc into AlN presents film development and fabrication challenges that increase with higher Sc content. To explore some of these challenges, AlScN lamb wave resonators (LWR) have been fabricated and demonstrated electromechanical coupling coefficients (k_t^2) over 10%. For $Al_{0.68}Sc_{0.32}N$ resonators at 40 MHz, unloaded quality factor (Q_u) reached values of 711 and k_t^2 of 10.28% when calculated from measured data. For resonators in the 400 MHz range, k_t^2 values reached 6.06% and Q_u of 890. Moving towards higher Sc-content, $Al_{0.6}Sc_{0.4}N$ 40% resonators show an increase in k_t^2 to 10% but a reduced Q_u of 400, and current efforts will attempt to understand and mitigate the mechanisms that cause this Q reduction. Other areas of focus include processing challenges such as significant curling of suspended devices from center to edge due to the sputter deposition process of AlScN, etching AlScN films with vertical sidewalls, and initiating high quality AlScN films on high-quality electrodes. Overcoming these challenges will enable high-coupling AlScN LWRs and other piezoelectric devices for future 5G and 6G applications. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

2:45 PM

(EMA-272-2022) Design and Modeling of Ferroelectric Based Switchable Multilayer Resonators for 5G Filters

W. Peng*[1]; S. Nam[1]; M. Zolfagharloo Koohi[2]; A. Mortazawi[1]

1. University of Michigan, Electrical and Computer Engineering, USA
2. Qorvo, R&D, USA

5G frontends need to support many new bands and sophisticated communication schemes, such as beamforming. Frontends using conventional implementations of passive filters require a lot more area to fully support filtering in 5G applications. Many applications impose high constraints to the area available to the frontend. Thin film bulk acoustic wave resonators utilizing ferroelectric materials are incorporated in a multilayer, multimode configuration that can be used to implement reconfigurable filters. The resonators can operate at multiples of the fundamental resonance frequency by only switching the polarity of the applied DC bias field while preserving electromechanical coupling. Therefore, such resonators can not only switch between modes but also operate beyond the frequency limitations of conventional FBARs without performance compromise. A novel modeling approach based on phenomenology of the ferroelectric materials is presented to account for the full response of the resonator under different electrical and mechanical conditions.

3:00 PM

(EMA-273-2022) Do $SrTiO_3$-$PbTiO_3$ superlattices exhibit negative permittivity?

F. Bergmann*[2]; B. T. Bosworth[2]; E. Marksz[2]; A. Hagerstrom[2]; S. Das[3]; R. Ramesh[3]; N. Orloff[1]

1. NIST, Communications Technology Laboratory, USA
2. NIST, USA
3. UCBerkeley, MSE/Physics, USA

We present recent results on broadband on-wafer permittivity measurements of $SrTiO_3$-$PbTiO_3$ superlattices up to 110 GHz. Polar vortices form in the ferroelectric $PbTiO_3$-phase of the superlattice. We recorded complex in-plane permittivity, horizontally and vertically to the vortex cores. We discuss evidence towards local negative permittivity.

3:15 PM

(EMA-274-2022) High-frequency Dielectric Characterization of BST-loaded, (Meth)acrylate-based Composites

M. K. Forstmeier*[1]; M. Yuan[2]; S. Perini[2]; M. Lanagan[3]; B. M. Foley[1]

1. The Pennsylvania State University, Mechanical Engineering, USA
2. The Pennsylvania State University, Materials Research Institute, USA
3. Penn State University, Dept. of Engineering Science and Mechanics, USA

The deployment of 5th-Generation (5G) and 6th-Generation (6G) networks will fundamentally change many aspects of our daily lives, including smart cities via the internet-of-things (IoT) and autonomous vehicles. These applications will require advanced materials and manufacturing methods to rapidly prototype, develop and supply the RF elements needed to bring the technology online. Our work presented here lies at the intersection of these material and manufacturing space, focused on the development of nanoparticle-loaded, methacrylate-based photoresin composites containing up to 30 vol % barium-strontium titanate (BST) to tune the relative permittivity. Disks of UV-cured material at various loading fractions of BST are fabricated via a casting process, and issues related to the use of highly-loaded composite resins in commercial stereolithography (SLA) printers are highlighted. The complex dielectric properties (relative permittivity and loss tangent) as a function of vol % BST are characterized in the W-band (75 – 110 GHz) using a transmission/reflection approach with the Swiss-to-12 dielectric test fixture and W-band frequency extension modules from Virginia Diodes, Inc (VDI) driven by a vector network analyzer. This work highlights the exciting potential for nano-loaded composites in the additive manufacturing space for RF applications.

4:00 PM

(EMA-275-2022) Modeling the relaxor dielectric dispersion of Ba 1−x Sr x TiO 3 with a local phase field method

A. Gurung[1]; J. Mangeri[2]; P. Alpay[3]; S. Nakhmanson*[3]

1. University of Connecticut, Physics, USA
2. Luxembourg Institute of Science and Technology, Materials Research and Technology Department, Luxembourg
3. University of Connecticut, Materials Science and Engineering, USA

The solid solution Ba 1−x Sr x TiO 3 (BST) displays dielectric response that is highly tunable, while also exhibiting low losses in a broad frequency regime, including microwave. Therefore, there is a need for better understanding of the influence of BST microstructure on its properties and performance in a variety of technological applications. Since local polarization in BST is strongly dependent on composition, so is its response to an applied AC field. In this work, we have adopted a phase field method to study the frequency dependent dielectric response of this system, while accounting for the local fluctuations in the solid-solution composition. By utilizing an energy function that includes a spatial dependence on averaged Ba content, we connected relaxor-like features in the dielectric dispersion to local spatial inhomogeneities, such as average size of Ba-rich regions, across a wide range of temperatures. These results show that the adopted simple coarse-grained approach to the relaxor problem is sensitive enough to reveal correlations between the frequency dependence of the dielectric response and modulations in the material morphology and microstructure.

4:15 PM

(EMA-276-2022) Multi-Phase Microwave Dielectric Materials for Applications in 5G Wireless Communications

M. D. Hill*[1]; S. Polisetty[1]

1. Trans-Tech, Inc., Research and Development, USA

Modern wireless communications require the use of specialized dielectric materials for applications including high frequency filters and patch antennas for planar antenna arrays for low earth orbit (LEO) satellite communications. The material requirements may include a temperature stable dielectric constant, a low loss tangent at frequencies above 3GHz at a chosen dielectric constant. While single phase materials have difficulty meeting all of these stringent requirements, a composite of two or three thermodynamically compatible phases will often be able to simultaneously meet all requirements at the desired dieelctric constant. Two phase combinations including rutile (titanium dioxide) are especially interesting due to its high dielectric constant (100) and low loss tangent. However, this adds another design challenge in that not all desirable microwave dielectric compositons are thermodynamically compatible with rutile. Data will be presented on specifically designed tetragonal tungsten bronze and spinel structured dielectrics which are end members for multi-phase polycrystalline ceramic bodies useful for 5G and other wireless applications.

4:30 PM

(EMA-277-2022) Industry Panel: Trends (Invited)

N. Orloff*[1]

1. NIST, Communications Technology Laboratory, USA

In this panel, we will discuss trends in industry. These trends include technology, standards, and measurement and more importantly how materials can help. Attendees can submit during the panel or ahead of time by emailing the session organizer. Each question will be read to the panelists and answered during the session. The industry panel is also a fantastic opportunity to provide technical feedback, speak broadly about new research directions, and identify basic research that can be driven by industry problems.

S13: Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics

Design of Electronic Materials I

Room: Citrus B

Session Chair: Mina Yoon, Oak Ridge National Laboratory

8:30 AM

(EMA-233-2022) Combining High Performance First Principles Computation, Monte-Carlo and Machine-Learning Methods for Statistical Mechanics of Materials (Invited)

M. Eisenbach*[1]

1. Oak Ridge National Laboratory, Center for Computational Sciences, USA

I will describe an approach to utilize machine learning to combine first principles density functional calculations with classical Monte-Carlo simulations to investigating the statistical mechanics of materials. Density functional calculations are a useful tool in the study of ground state properties of materials. The investigation of finite temperature properties on the other hand often relies on empirical models that allow the large number of evaluations of the system's Hamiltonian that are required to sample the phase space needed to obtain physical observables as function of temperature. We demonstrate a solution that harnesses the power of massively parallel computers by combining classical Monte-Carlo calculations with our highly scalable electronic structure code (LSMS) by employing Machine Learning techniques. The combination of first principles calculations with a machine learning workflow, that can consider both classical interaction models and artificial neural network based models, allows us to investigate alloy ordering transitions for increased simulation cell sizes. Our approach is able to sample both magnetic or sample chemical order, allowing the first principles calculation of order/disorder phase transitions and phase separations in alloys. We will present our method as well as results for ordering transitions in alloys.

9:00 AM

(EMA-234-2022) Enhancing the bond valence representation for prescreening of solid state ionic conductors (Invited)

K. Kameda[1]; T. Ariga[1]; S. Manzhos*[1]; M. Ihara[1]

1. Tokyo Institute of Technology, School of Materials and Chemical Technology, Japan

Solid state ionic conductors are important, in particular, for the development of electrochemical batteries and fuel cells. Computational prescreening and selection of such materials is promising to help discover novel ionic conductors but is also challenging due to the high cost of electronic structure calculations which would be needed to properly assess the properties of interest such as material's stability and ion diffusion barrier or rate, in partucular in the presence of multiple possible difffusion paths. The bond valence approach is enticing for this application as it allows for rapid prescreening among multiple compositions and structures, but the simplicity of the approximation can make the results unviable. We will present the results of exloring the approach of refitting the parameters of the bond valence model based on molecular dynamics and density functional theory simulations, to facilitate prescreening of mixed oxide candidates for proton and oxygen ionic conductors.

9:30 AM

(EMA-235-2022) Accelerating Simulations-Assisted Materials Design Using Machine Learning (Invited)

W. Saidi*[1]

1. University of Pittsburgh, Materials Science, USA

"Computational experiments" have emerged as a powerful complement to experiment in the design of new materials. While structure-property relationships can be accurately determined using density functional theory (DFT), these calculations are computationally demanding, limiting their use in screening a large set of candidate structures. The development of statistical tools based on machine learning (ML) and deep networks in conjunction with database construction and data mining have been demonstrated to significantly boost these quantum mechanical approaches. In the first part of this talk, recent progress in utilizing ML for computational design and discovery of novel hybrid perovskites and high entropy alloy catalysts will be reviewed, highlighting the need to utilize well-designed hierarchical ML architecture to obtain a higher prediction fidelity. The second part of the talk will describe our recent methodological developments for generating ML potentials (MLPs), demonstrating that MLP-based material property predictions converge faster with respect to precision for Brillouin zone integrations than DFT-based property predictions. Statistical error metrics to accurately determine a priori the precision level required of DFT training datasets for MLPs will be presented, thus significantly reducing the computational expense of MLP development.

10:30 AM

(EMA-236-2022) Data-Enhanced Multiscale Theory of Operando Energy Conversion Systems (Invited)

K. Reuter*[1]

1. Fritz Haber Institute of the Max Planck Society, Germany

Emerging operando spectroscopies and microscopies reveal a highly dynamic behavior of interfaces in energy conversion systems. Insufficient insight and the concomitant inability to control or exploit the corresponding strong structural and compositional modifications centrally limits the development of performance catalysts, electrolyzers or batteries required for a sustainable energy supply for our society. Predictive-quality modeling and simulation has become a major contributor to accelerated design all across the materials sciences, not least through powerful computational screening approaches. Current first-principles based methodology is nevertheless essentially unable to address the substantial, complex and continuous morphological transitions at working interfaces. I will review this context from the perspective of first-principles based multiscale modeling, highlighting that the fusion with modern machine learning approaches is key to tackle the true complexity of working systems. Approaches pursued by our group thereby aim at maximum data efficiency by exploiting physical models wherever possible or through active learning that only queries data on demand. Illustrative examples will be drawn from thermal methanation catalysis, electrocatalytic oxygen evolution and organic semiconductor photovoltaics.

11:00 AM

(EMA-237-2022) ML Assisted Discovery of Electronic and Energy Materials (Invited)

A. K. Singh*[1]

1. Indian Institute of Science, Materials Research Centre, India

Data driven machine learning methods are emerging as one of the promising tools for expanding the discovery domain of materials to unravel useful knowledge. The power of these methods will be illustrated by covering three major aspects, namely, development of prediction models, establishment of hidden connections and scope of new algorithmic developments. For, we have developed accurate

prediction models for various computationally expensive physical properties such as band gap, band edges and lattice thermal conductivity. These models are developed with GW level accuracy, and hence can accelerate the screening of desired materials by estimating the band gaps and band edges. For the lattice thermal conductivity prediction model, an exhaustive database of bulk materials is prepared. The performance of the ML model for thermal conductivity is far superior than the physics-based Slack model, highlighting the simplicity and power of the proposed machine learning models. For the second aspect, we have connected the otherwise independent electronic and thermal transport properties. An accurate machine learning model for thermal transport properties is proposed, where electronic transport and bonding characteristics are employed as descriptors. In the third aspect, we have proposed a new algorithm to develop highly transferable prediction models.

11:30 AM

(EMA-238-2022) Machine Learning enabled Prediction of Adiabatic Temperature Change in Lead-Free $BaTiO_3$-based Electrocaloric Ceramics

M. Su*[3]; R. Grimes[3]; S. Garg[1]; D. Xue[2]; P. Balachandran[3]

1. Birla Institute of Technology and Science, India
2. Xi'an Jiaotong University, China
3. University of Virginia, USA

In this paper, we develop a data-driven machine learning (ML) approach to predict the adiabatic temperature change (ΔT) in $BaTiO_3$-based ceramics as a function of chemical composition, temperature, and applied electric field. The data set was curated from a survey of published electrocaloric measurements. Each chemical composition was represented by elemental descriptors of A-site and B-site elements. Pair-wise statistical correlation analysis was used to remove linearly correlated descriptors. We train two separate regression-based ML models for indirect and direct measurements and found that both are able to capture the general trend of the Temperature vs. ΔT curve for various applied fields. We then complement the regression models with a classification learning model that predicts the expected phase as a function of chemical composition and temperature. Both regression models predict a global maximum in ΔT near a Tetragonal to Cubic or Rhombohedral to Cubic phase transition. The regression and classification learning models work together to help identify promising $BaTiO_3$-based ceramics candidates for electrocaloric applications. An interactive, open source web application is also developed for the interested researchers to query our trained models and rapidly predict ΔT as a function of chemical composition.

11:45 AM

(EMA-239-2022) The effect of strain and boundary states on the electronic and topological properties ultrathin Bi_2Se_3

S. Kang*[1]; W. Ko[1]; M. Brahlek[2]; R. Moore[2]; M. Yoon[2]

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

Bismuth selenide (Bi_2Se_3) is a well-known material as a quantum spin Hall insulator (QSHI) with Dirac surface states protected by time-reversal symmetry. Recently, some screw dislocations in Bi_2Se_3 with their electronic properties have been observed by Scanning tunneling microscopy (STM) and Scanning tunneling spectroscopy (STS). Based on first-principles calculations and tight-binding approaches, we present the thickness-dependent strain effect and the boundary state at the step edge of a QSHI to evaluate the dislocation effect. It is shown that the connected boundary states between topological surface states at the step edge is thickness dependent. Our results describe well the experimental observation of the changes in bandgap as a function of film thickness at the step edge. We also discover that strain induces the quantum phase transition from normal insulator to topological metal in a few quintuple layers. This implies that the topological properties can be easily controlled by applying strain. Acknowledgement: This work was supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Quantum Science Center by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES), Materials Sciences, and Engineering Division

12:00 PM

(EMA-240-2022) Deep learning enabled design of optoelectronic organic materials and hybrid organic-inorganic interfaces (Invited)

R. Maurer*[1]

1. University of Warwick, Department of Chemistry, United Kingdom

Materials for organic light emitting diodes need to satisfy various conditions to be used in cost effective and efficient devices. Materials need tailored optoelectronic properties and be synthetically viable. As devices are composed of organic thin films with different functionality, the optoelectronic properties of materials need to be design in concert and the role of the interfaces between films must be understood. Computational high-throughput screening of molecular excited states can greatly facilitate this complex multi-objective design problem. I will present our recent work on deep machine learning models that are able to predict structure, molecular electronic structure, and excited states of organic molecules and metal-organic interfaces. Our models predict optical excitations, the fundamental gap, electron affinity and ionisation potential for large organic molecules of diverse composition. While the models are trained on first principles electronic structure data, the prediction process requires no recourse to computationally expensive ab initio calculations. The accuracy and transferability of the models can be assessed against photoemission spectroscopy data. I will further showcase how such models can be used in combination with generative machine learning to discover novel organic compound combinations that satisfy specific optoelectronic properties.

12:30 PM

(EMA-241-2022) High-throughput first-principles exploration of 2D-tin structures and their topological properties

M. Yoon[1]; S. Yeom*[2]

1. Oak Ridge National Laboratory, USA
2. University of Tennessee, Department of Physics and Astrononmy, USA

Stanene (2D Sn) is a promising material for nanoelectronics or quantum computing because it is a proposed topological insulator (TI) at the room temperature. Because electrons can travel on the edges of these TIs without heat dissipation, this could greatly increase the efficiency and performance of electronic devices. We explored the (meta)stable structures of 2D Sn using our automated high-throughput workflow that combines first-principles calculations and particle swarm optimization and identified new structures of 2D Sn with different electronic and topological properties. We also found that substrates play a critical role in the stability of 2D Sn structures with versatile properties. Our findings should be instrumental for the experimental development of new 2D Sn with desirable properties.

12:45 PM

(EMA-242-2022) Finding ferroelectric polarization from STEM and STM images

A. Ghosh*[1]; C. T. Nelson[1]; M. Oxley[1]; X. Zhang[2]; M. Ziatdinov[1]; I. Takeuchi[2]; S. Kalinin[1]

1. Oak Ridge National Laboratory, USA
2. University of Maryland, USA

Scanning transmission electron microscopy (STEM) has become an important tool for studying atomic structures of complex materials with picometer precision and the associated order parameter fields. The process of finding polarization values via preprocessing images to remove noise and instrumental distortions, find positions of all the observed atomic columns corresponding and calculate atomic displacements is laborious. In this work, we have proposed an alternate approach of utilizing deep convolution neural networks (DCNNs) for direct polarization mapping from STEM data. The DCNN is trained on the manually-labeled part of the images and the training data is constructed using image patches (parts of original images cropped for a specific window size) generated with and without information about atomic positions, creating the local feature set. We have demonstrated this workflow for predicting polarization maps without atom-finding for STEM images with different Sm dopant concentrations in $BiFeO_3$, such that the explored feature space encompasses both ferroelectric and weakly-ferroelectric systems. This approach is extendible to Scanning Tunneling Microscopy (STM/S) datasets of quantum materials to study other functionalities such as superconducting gap or the intensity of selected quasiparticle interference spots.

Design of Electronic Materials II

Room: Citrus B

Session Chair: Mina Yoon, Oak Ridge National Laboratory

2:00 PM

(EMA-278-2022) AI-Driven Design of High Entropy Halide Perovskite Alloys (Invited)

A. Mannodi-Kanakkithodi*[1]

1. Purdue University, Materials Engineering, USA

Halide perovskites with desirable stability, electronic structure, and optical absorption are sought for solar cells, electronic devices, infrared sensors and quantum computing. Compositional manipulation via alloying at cation or anion sites, or via incorporation of point defects and impurities, can help tune their properties. In this work, we develop AI-based frameworks for the on-demand prediction and optimization of the phase stability, band gap, optical absorption spectra, photovoltaic figures of merit, and defect formation energies for a chemical space of ABX_3 halide perovskites with several choices for A, B and X, mixing allowed at each site, and several possible crystal structures. These frameworks are powered by high-throughput density functional theory (DFT) computations, unique encoding of atom-composition-structure (ACS) information, and rigorous training of advanced neural network (NN)-based predictive models and genetic algorithm-based multi-objective optimization frameworks. Multi-fidelity learning is applied to bridge the gap between low accuracy calculations and high-fidelity data, constituted of expensive computations or collected experimental measurements. AI-based recommendations are synergistically coupled with targeted synthesis and characterization, leading to successful validation and discovery of novel halide perovskite compositions for improved performance in solar cells.

2:30 PM

(EMA-279-2022) Data analytics accelerates the experimental discovery of new thermoelectric materials with extremely high figure of merit

Y. Zhong[2]; X. Hu[3]; D. Sarker[1]; Q. Xia[2]; C. Yang[2]; L. Xu[4]; Z. Han*[1]; S. Levchenko[1]; J. Cui[2]

1. Skolkovo Institute of Science and Technology, Russian Federation
2. Ningbo University of Technology, School of Materials and Chemical Engineering, China
3. Fritz Haber Institute of the Max Planck Society, Germany
4. Hanyang University, Department of Electrical and Biomedical Engineering, Republic of Korea

Thermoelectric (TE) materials are among very few sustainable yet feasible energy solutions of present time. This huge promise of energy harvesting is contingent on identifying/designing materials having higher efficiency than presently available ones. However, due to the vastness of the chemical space of materials, only its small fraction was scanned experimentally and/or computationally so far. Employing a compressed-sensing based symbolic regression in an active-learning framework, we have not only identified a trend in materials' compositions for superior TE performance, but have also predicted and experimentally synthesized several extremely high performing novel TE materials. Among these, we found polycrystalline p-type $Cu_{0.45}Ag_{0.55}GaTe_2$ to possess an experimental figure of merit as high as ~2.8 at 827 K. This is a breakthrough in the field, because all previously known thermoelectric materials with a comparable figure of merit are either unstable or much more difficult to synthesize, rendering them unusable in large-scale applications. The presented methodology demonstrates the importance and tremendous potential of physically informed descriptors in material science, in particular for relatively small data sets typically available from experiments at well-controlled conditions.

2:45 PM

(EMA-280-2022) Experimental discovery of structure-property relationships in ferroelectric materials via active learning (Invited)

Y. Liu*[1]; K. Kelley[2]; R. Vasudevan[1]; H. Funakubo[3]; S. Trolier-McKinstry[4]; M. Ziatdinov[1]; S. Kalinin[5]

1. Oak Ridge National Lab, USA
2. Oak Ridge National Lab, Center for Nanophase Materials Sciences, USA
3. Tokyo Institute of Technology, Japan
4. Pennsylvania State University, Materials Science and Engineering, USA
5. Oak Ridge National Lab, USA

The functionalities of topological and structural defects in ferroelectric materials including domain wall (DW) dynamics, conductivity of topological defects, and light induced phenomena have been a source of much fascination in condensed matter physics. Until now, the search for interesting functionalities has been guided by auxiliary information from scanning probe microscopy (SPM) to identify potential objects of interest based on human intuition. Here, we developed a machine learning (ML) driven SPM workflow that actively discovers relationships between domain structure and functional responses (hysteresis, I-V curves, non-linearities), which combines the power of ML methods to learn the correlative relationships between high dimensional data, and human-based physics insights encoded in the acquisition function. This approach demonstrates that the discovery path and sampling points of on-field and off-field hysteresis loops are largely different. The larger polarization mobility in the vicinity of 180° DWs leads to more significant hysteresis loop opening in on-field measurements, while off-field measurements only detect slowly relaxing components due to strong

pinning at ferroelastic DWs. This approach can be apated to apply to a broad range of imaging and spectroscopy methods, e.g., SPM, electron microscopy, optical microscopy, and chemical imaging.

3:45 PM

(EMA-281-2022) AtomAI for deep learning for microscopic images

A. Ghosh*[1]; S. Kalinin[1]; M. Ziatdinov[1]

1. Oak Ridge National Laboratory, USA

In the past couple of decades, the development and availability of more computational capabilities including accessible CPU/GPUs, efficient algorithms, and corresponding implementations have significantly advanced the field of physical simulations at different length scales. The electron and scanning probe microscopies have also emerged as keystone tools for the exploration of matter on the atomic and mesoscale levels. However, the utilization of theoretical models to guide, perform experiments and refine the parameters in both spaces, to establish a continuous feedback-loop, are still at an early stage. Subsequently, there is a need to bridge this gap to allow for the co-navigation of theory and experiment for development of comprehensive physics of materials. AtomAI open-source software which is a Python-based infrastructure aims at establishing a bridge environment between the instrument-specific libraries and general physical analysis by enabling the seamless deployment of the deep learning algorithms including deep convolutional neural networks and invariant variational autoencoders to image and hyperspectral data and transforming the experimental knowledge to build suitable environments for performing atomistic simulations.

4:00 PM

(EMA-282-2022) Scalable fabrication and microstructure optimization of garnet-based ceramic components (Invited)

D. Fattakhova-Rohlfing*[1]

1. Forschungszentrum Juelich, Institute of energy and climate reasearch (IEK-1), Germany

All-solid-state batteries based on garnet $Li_7La_3Zr_2O_{12}$ (LLZO) electrolytes face several challenges to fully utilize their potential with respect to intrinsic safety and high energy density. Particularly, the integration of solid electrolyte powders in the cell components and the scalable fabrication of cell designs providing maximum energy density on the cell level remain important issues to be addressed. I will discuss the fabrication of critical components of garnet-based cells, namely freestanding LLZO separators and LLZO-containing ceramic cathodes, with a special focus on understanding and controlling the factors influencing the grain boundary properties. I will demonstrate how the alteration of the LLZO powder surface due to Li+/H+-exchange during various manufacturing steps affects the processability and the electrochemical performance of tape-cast LLZO separators, and will present the ways to produce thin, dense, free standing LLZO separators with significantly improved total Li-ion conductivity and increased critical current density. Furthermore, I will show the importance of LLZO surface control also for the fabrication of the cathode layers, and will address the microstructure control and processing optimization as efficient means to obtain all-ceramic cathode layers with a high loading of cathode active material, high capacity utilization and improved cycling stability.

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*** Denotes Presenter**

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