The 32nd Rio Grande Symposium on Advanced Materials

Monday, October 24th, 2022

Embassy Suites
Albuquerque, NM

The 32nd Rio Grande Symposium is Sponsored by

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7:30	**Registration and Exhibition - Pre Con Hallway**			
8:00 - 9:00	**Continental Breakfast - Sandia Ballroom IV**			
Room	Piñon	Sandia Ballroom VI	Sandia Ballroom VII	Sandia Ballroom VIII
8:45	Theory and Modeling (9:00 AM)	Electronics, Magnetics and Photonic Materials & Devices (9:00 AM)	Structural Materials and Failure Mechanisms	Biomaterials and Soft Materials
10:45	**Break**			
11:00	**Kreidl Memorial Lecture, Professor Rajendra Bordia - (Sandia Ballroom V, Lunch Provided)**			
Room	Piñon	Sandia Ballroom VI	Sandia Ballroom VII	Sandia Ballroom VIII
1:00	Theory and Modeling	Electronics Magnetics and Photonic Materials Devices / Energy Nuclear Materials	Structural Materials and Failure Mechanisms	Advanced and printed Manufacturing
2:15	**Break / Refreshments**			
2:30	Theory and Modeling / Low Dimension 2D Materials	Energy Nuclear Materials	Other Advanced Materials	Advanced and Printed Manufacturing
4:00	**Poster – Pre-Con Hallway**			
5:15	**End / Award Announcements**			

In Memorium

Norbert J. Kreidl, 1904–1994

Norbert J. Kreidl died July 11, 1994, in Liechtenstein just after his 90th birthday. A native of Austria, he received a Ph.D. in physics from the University of Vienna in 1928. After a year of silicate research at the Kaiser Wilhelm Institute, he became involved with the glass industry in Czechoslovakia.

In 1938 he immigrated to the United States to become assistant professor of glass technology at Pennsylvania State University. While at Penn State, he served as a consultant to Bausch & Lomb Optical Co., joining the company in 1943 and rising to the position of director of materials R&D. After 25 years, he retired and began a second career, teaching—first at Rutgers University and then at the University of Missouri-Rolla. He was a Fulbright Professor at Vienna during 1972–73 and again during 1976–77.

After retiring in 1974 as professor emeritus of ceramic engineering at Rolla, he moved to Santa Fe, N.M., and continued teaching part-time. In 1981, he became a partner, vice president and secretary of Materials Technology Associates Inc.

Kreidl is best known for his work on the optical properties of glass, with color and radiation effects being a particular focus. His work resulted in the creation of many optical and ophthalmic glasses, including novel aluminate glasses. His research on compositions for sunglasses led to a continuing interest in the colors resulting from redox interactions with iron and other minor constituents in the base glasses.

Eventually, he expanded these studies to include radiation-induced damage in glass, radiation-resistant glasses, dosimeter glasses, and slow neutron scintillation glasses. Overall, his work led to the publication of more than 150 technical papers and 10 patents.

A member of The American Ceramic Society since 1939, he made many substantial contributions to its growth. He was an energetic participant in the Glass & Optical Materials Division, serving as chair in 1953 and as trustee during 1962–65. Many national and international awards recognized his research and his skillful leadership. Society awards include: Fellow, 1951; Toledo Glass & Ceramic Award, 1966; John Jeppson Medal and Award, 1969; Distinguished Life Member, 1991; and George W. Morey Award, 1992.

Kreidl held honorary doctorates from Alfred University, the University of Vienna and the Friedrich Schiller University in Jena, and was an honorary fellow of the Society of Glass Technology. At the time of his death, he was an adjunct professor at both the University of Arizona and the University of New Mexico.

He was a familiar figure at glass meetings throughout the world. An active, stimulating presence, he organized symposia in new fields of glass and skillfully moderated technical debates, astutely pointing out similarities and differences between the points of view.

Norbert J. Kreidl

Kreidl was a major link between the ACerS and the International Commission on Glass (ICG). Having attended the First International Congress on Glass in Milan and Venice in 1933, he had a personal association with the history of the ICG and a keen sense of the great opportunities it offered for bringing together glass scientists and engineers from all over the world.

In fact, he led the U.S. delegation to the Third Congress in 1953 and represented the United States on the ICG Steering Committee from 1952 to 1963. A member of the committee that drafted the new ICG constitution in the 1960s, he served as vice president during 1966–69 and as president during 1969–72.

No observations on Kreidl's accomplishments would be complete without stating that they were always done with sensitivity to the feelings of others, a clear vision of what would work and an excellent sense of humor. In recognition of his lifelong dedication to helping young scientists and engineers, the Glass & Optical Materials Division of ACerS established the Norbert J. Kreidl Award for Young Scholars in 1990. The words at the dedication of this award are a fitting epitaph for his remarkable man:

> "He brings to our meetings encouragement, support and incisive questions which always provide us with a new perspective and a bridge to established understanding. His encyclopedic knowledge of glass is always available to those who ask. He provides a rich resource to those of us who have the good fortune to know him and who have benefited by his presence . . . ."

For those who may wish to express their condolences, Kreidl's widow, Melanie Kreidl, resides at 1433 Canyon Road, Santa Fe, NM 87501. She has requested than any memorial contributions be donated to the Norbert J. Kreidl Award, c/o Peter C. Schultz, Heraeus Amersil, 3473 Satellite Blvd., Suite 300, Duluth, GA 30136.

The undersigned and all of Kreidl's friends around the world want to extend in memorium our heartfelt thanks to a great scientist and a wonderful human being. We are pleased to acknowledge our debt to Kreidl, our esteemed mentor, and to express our gratitude for being included in his extended family. To Melanie, we say a special thanks for sharing him with us so generously. You will be in our thoughts and in our prayers.

- J. Raymond Hensler
- William R. Prindle
- Peter C. Schultz
- Stephen D. Stoddard
- Donald R. Uhlmann

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Rajendra K. Bordia
George J. Bishop III Chair Professor
of Ceramics and Engineering, Clemson University

Professor Rajendra Bordia is the George J. Bishop, III Professor of Materials Science and Engineering at Clemson University in Clemson, SC, USA. He is also the Scientific Director of Materials Assembly and Design Excellence in South Carolina (MADE in SC) – an NSF funded EPSCoR Track I Research Infrastructure Improvement Award. From 2013 to February 2019, he was the Chair of his Department. He was a faculty member at the University of Washington (1991-2013) and a Research Scientist in DuPont Co. (1986 to 1991). He received his B.Tech from IIT, Kanpur, India (1979), and his M.S. (1981) and Ph.D. (1986) from Cornell University, Ithaca, NY, USA.

His research is at the intersection of materials and mechanics and is focused on fundamental and applied studies in the processing and properties of complex material systems for energy, extreme environment and medical applications. He has authored or co-authored over 170 peer-reviewed technical publications.

He was elected Fellow of the American Ceramic Society (2002); Fellow of the Indian Institute of Metals (2010); and academician in the World Academy of Ceramics (2012). Other significant awards include: Humboldt Research award from the Alexander von Humboldt Foundation, Germany (2007); and the Outstanding Educator Award of the American Ceramic Society (2012). He is an Associate Editor of the Journal of the American Ceramic Society (1988-Present); and Editor-in-Chief of the Ceramics International (2009 – Present). He has been elected to serve as the President of the American Ceramic Society during the 2023-2024 year.

Kreidl Lecture Abstract

Analysis and Simulation Guided Process and Properties of Anisotropic Hierarchical Porous Ceramics for Energy Conversion and Storage

Our current research is focused on developing processing strategies to control the microstructure of ceramics at different length scales. One of the focal areas porous ceramics produced by controlled sintering of powder compacts. Many of the applications of porous ceramics demand optimization of a multitude of properties some of which have conflicting requirements on the microstructure. Materials with designed anisotropic and/or hierarchical microstructures have the potential to optimally address the requirements.

We will first present a broad overview of the use of porous ceramics in advanced energy conversion and storage applications including the property requirements. Next, we will present results from our collaborative projects focused on microstructural control in hierarchical and/or anisotropic porous ceramics. Porous ceramics are used in a broad range of technologies of interest to energy conversion and storage including electrochemical applications like electrodes for solid oxide fuel cells, high temperature insulators, thermal energy storage and electrochemical energy storage. In these applications, a multitude of properties are of interest. For specific applications, a subset of mechanical, thermal, electrical and ionic conductivity, gas diffusion and chemical reactivity need to be optimized. In this presentation, results will be presented on the processing approaches to make these designed microstructures, the quantification of the 3D microstructure at different length scales and simulations to design optimal microstructures for specific applications including electrodes for solid oxide fuel cells and electrolysis cells, and Li-ion batteries

The research in the is supported by the US National Science Foundation

Theory and Modeling

Room: Piñon
Session Chair: Deep Choudhuri, New Mexico Tech

9:00 AM

Physics-based modeling of reactive charge-transfer in complex molecules and materials (Invited)

Susan Atlas*[1]
1. Department of Chemistry and Chemical Biology and Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131

Atomistic simulation is an essential tool for exploring the energy landscapes and energy-entropy tradeoffs in designed structural materials and heterogeneous biophysical systems. Recent advances in empirical machine learning models continue to expand the classes and complexity of systems that can studied through the parametrization of empirical force fields. However, for complex materials such as high-entropy alloys or oxide materials supporting multiple valence charge states as a function of local chemical environment, it is challenging to span the complete space of chemical interactions with empirically-fitted interaction potentials and limited training datasets. We describe a physics-based, atomistic force field, the ensemble DFT charge-transfer embedded-atom method (ECT-EAM), that formally couples the electronic and atomistic length scales through an ensemble density functional theory reformulation1,2 of the original embedded-atom model for elemental metals. Charge transfer is expressed in terms of ensembles of ionic state basis densities of individual atoms, and charge polarization, in terms of atomic excited state basis densities. This provides a compact yet flexible representation of atomic interactions, encompassing both local and system-wide effects. Charge rearrangement is realized through the evolution of ensemble weights, adjusted at each dynamical time step via chemical potential equalization.

Acknowledgements: NSF, DoD/DTRA CB Basic Research Program (Grant No. HDTRA1-09-1-0018).

[1] K Muralidharan, SM Valone, and SR Atlas. arXiv:cond-mat/0705.0857v1 (2007).

[2] SR Atlas. J. Phys. Chem. A 125, 3760â˘'3775 (2021)

9:30 AM

First-principles exploration of diffusion activation energy in CoCrNi and CoCrFeMnNi high-entropy alloys, with comparison to creep activation energy

Chris Lafferty*[1], Dr. Chelsey Hargather[1]
1. New Mexico Institute Of Mining and Technology

High-entropy alloys (HEAs) are potential materials candidates for high performance engineering applications because of their exceptional combinations of strength and ductility. HEAs are defined as an alloy made of five or more elements, in equal proportion, which often form a single solid solution phase. Due to the difficulty involved in modeling single phase solid solutions, atomistic calculations are computed using density functional theory with special quasirandom structures (SQS) to represent the arrangement of atoms for analysis. In the present work, properties related to creep failure are investigated in the CoCrFeMnNi HEA and its constituent ternary systems. Vacancy formation energy is calculated by removing each type of atom present in the HEA, and the vacancy formation energy calculated is compared to literature and the pure systems. Chemical potentials are calculated for each type of atom migrating into the neighboring vacancy, and then compared to literature and pure system chemical potentials. Finally, the differences in magnetic and non-magnetic calculations are explored. Once the methods of this work are validated against current methods in the literature, the same methods will be done to analyze a similar yet less studied system (CoCrCuFeNi).

9:45 AM

Investigation of in-liquid ordering mediated transformations in Al-Sc via *ab initio* molecular dynamics and unsupervised learning

Deep Choudhuri*[1], Bhaskar Majumdar[1], Hunter Wilkinson[1]
1. New Mexico Tech

Scandium is well-known to produce grain refinement in Al-based alloys, and it's potency is generally attributed to intermetallic Al3Sc formation within liquid phase. However, the influence of Sc atoms and Al3Sc on the local structure of the surrounding melt, and subsequent nucleation remains unclear. Towards that end, we have probed structural changes in three bulk-compositions, i.e. Al-xSc (x=0, 0.4,1.0at.%), and near liquid-Al/Al3Sc interfacial regions using *ab initio* molecular dynamics. In-liquid ordering was determined using unsupervised learning techniques, i.e., structural fingerprinting, dimensionality reduction, and cluster analysis. Sc atoms ordered the surrounding liquid Al atoms by forming Sc-centered polyhedrons, while liquid-Al/Al3Sc interface manifested planar ordering that resembled {100}*fcc*−Al. Both structures were geometrically persistent but constitutionally transient, i.e., they exchanged Al atoms with the surrounding liquid. At a lower temperature, {100}*fcc*−Al interfacial planes heteroepitaxially nucleated equilibrium *fcc*-Al, while Sc-centered polyhedrons sequentially formed metastable *hcp*- and *bcc*-Al. Using our simulations and extant experimental reports, we postulate two transformation pathways during Al-Sc solidification: (i) Sc−centered polyhedrons → Al3Sc → liquid−Al/Al3Sc interfacial ordering → *fcc*−Al; and (ii) Sc−centered polyhedrons → *hcp*−Al → *bcc*−Al → *fcc*−Al. The two in-liquid ordered structures provide an atomistic basis for the potency of Sc element, and, also, serve as possible structural metrics for designing novel Al-based alloys.

10:00 AM

Experimentally Informed Model Development of Glass-Ceramic Materials

Brian Lester*[1], Kevin Strong[1], Thomas Diebold[1], John Laing[1], Steve Dai[1], Kevin Long[1],
1. Sandia National Laboratories

Glass-ceramics are an exciting material for a variety of biomedical and sealing applications. This is due to a unique non-linear thermomechanical response arising from a novel combination of a heterogeneous microstructure and multiple inelastic constituents including an inorganic glass matrix and phase transforming silica polymorphs.

The application of these materials in seal and other applications requires the ability to be able to predict and analyze their thermomechanical behavior. Prior experimental work has focused primarily on their sealing ability and limited work has been done on combined thermal-mechanical loadings. This lack of data also means that relatively limited modeling attempts have been pursued.

In the current work, a new experimental campaign is pursued to characterize the thermomechanical (actuation) response and develop a novel 3D phenomenological model incorporating combined viscoelasticity and phase transformation. A novel thermomechanical load frame is developed and used to fill in the data gaps. These results are leveraged in the model development. Both experimental results and corresponding simulations are presented.

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10:15 AM

Formation of Secondary Gas Species During Acid Gas Adsorption in Rare-Earth Metal-Organic Frameworks

Matthew Christian*[1], Tina Nenoff[1], Jessica Rimsza[1]
1. Geochemistry Department, Sandia National Labortories
2. Material, Physical and Chemical Sciences Center

Rare-earth (RE) 2,5-dihydroxyterepthalic (DOBDC) based metal-organic frameworks (MOFs) are promising candidates for acid gas separations and adsorption from flue gas streams. However, previous simulations have shown that acid gases (H2O, NO2, and SO2) can react with the DOBDC ligand by deprotonating a hydroxyl group, protonating the acid gas. The protonation of NO2 to form HONO has been noted in several studies, but its presence is challenging to detect experimentally. Computational approaches can provide insight into the likelihood of secondary gas formation. Here, reaction barriers and formation energies of secondary protonated acid gases were evaluated by using both density-functional theory (DFT) and correlated wave-function methods. The relative stabilities of secondary gases and formation reaction energies were evaluated to reveal the likelihood of selected acid gases would react with the DOBDC MOF linker. Results of these calculations indicate how MOF stabilities in flue gas streams could be improved.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2022-11433 A

10:30 AM

Particle Processing: Recent Developments Implementing Particle-based Simulations

Leonardo E. Silbert*[1], Ishan Srivastava[1], Joseph M. Monti[1], Gary S. Grest[1], Jeremy B. Lechman[1],
1. School of Math, Science, and Engineering, Central New Mexico Community College
2. Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory
3. Sandia National Laboratories (Albuquerque)

The handling, transport, and packing of granular materials has broad relevance, spanning from geophysical phenomena, such as avalanches and sand dune formation, to industrial and defense applications, through powder technology, additive manufacturing, and the mechanics of soil and construction materials. While the study of monodisperse spheres has progressed significantly over the past two decades, here we explore more recent developments that allow us to extend computer simulation studies to systems that more closely relate to real-world and experimental systems. These include the capability to study systems with a high degree of particle size dispersity, non-spherical, complex, and frictional particle shapes, that can pack or flow in different geometries. We illustrate these newer capabilities with the study of the inclined plane flow of rod-like structures, and how the flow behavior depends on the size of the flowing pile and the frictional roughness between the rods.

10:45 AM

Break

Electronics, Magnetics and Photonic Materials & Devices

Room: Sandia Ballroom VI
Session Chair: Bryan Kaehr, Sandia National Labs

9:00 AM

Functional MEMS Compatible Thin Film Piezoelectric Research: Paving the Way for the Future (Invited)

Nathan Jackson*[1]
1. University of New Mexico, Mechanical Engineering Department and Center for High Technology Materials

Functional materials are the backbone of any Microsystem or MEMS transducer. My research at UNM focuses primarily on thin film piezoelectrics and magnetic films. My talk will focus on two different types of thin film piezoelectric materials, 1) flexible polymer composites and 2) novel doped Aluminum Nitride (AlN) films as a more stable alternative to ScAlN. Flexible polymer piezoelectric materials are in high demand due to wearable technology industry, however most polymer piezoelectrics are not compatible with current standard microfabrication techniques due to their low Curie Temperature. Our research has focused on creating new films that are microfabrication compatible with high spatial resolution and enhanced manufacturing capabilities. To accomplish this, we developed composites using nanoparticles of lead zirconate titanate (PZT), ZnO, and BaTiO3 using photopatternable SU-8 polymer and high temperature low CTE polyimide as the polymer matrix. In addition, we created electrically conducting polymer composites to create an all-organic polymer MEMS device. Using density functional theory, we have identified potential alternatives to Sc to create a more stable high piezoelectric thin film doped AlN material. TiAlN was experimentally tested and used to validate the DFT model which demonstrated a significant increase in d33 piezoelectric coefficient. The work presented has potential to lead to ground-breaking technology which could help enhance MEMS device performance.

9:30 AM

Novel Antiferromagnetic FeTe2 Phase Formation at the Sb2Te3/Ni80Fe20 Interface

Alexandria Will-Cole*[1]
1. Northeastern University (Boston, MA)
2. Sandia National Laboratories (ABQ, NM)

Topological insulators (TIs), specifically Bi1-xSbx alloys and van der Waals chalcogenides X2Q3 (X = Bi, Sb, Bi1-xSbx; Q = Se, Te) with tetradymite structure, have insulating bulk state and two-dimensional metallic surfaces enabled by topologically protected Dirac surface states.1-3 TIs exhibit large charge-to-spin conversion efficiencies, strong spin-momentum locking, and conductive surface states making them ideal for applications in spin-orbit-torque magnetic random access memory magnetic tunnel junction devices.4-10 Bilayer topological insulator/ferromagnet heterostructures are promising for spintronic memory applications due to their low switching energy and therefore power efficiency.4 Until recently, the reactivity of topological insulators with ferromagnetic films was overlooked in the spin-orbit-torque literature,9,11.12 even though there are reports that it is energetically favorable for topological insulators to react with transition metals and form interfacial layers.13-15 The novel intrinsic topological insulator phase NiBi2Te4 was recently reported at the interface of Bi2Te3/Ni80Fe20 â€“ thus these interfaces can host exciting new topological phases.15 Here we fabricated a bilayer topological insulator/ferromagnet heterostructure comprised of molecular beam epitaxy grown Sb2Te3 and DC sputtered Ni80Fe20. Broadband ferromagnetic resonance revealed spin-pumping evident by significant enhancement in Gilbert damping and the reduction of the effective magnetization likely a signature of the topological surface states or the presence of large spin-orbit-coupling in the adjacent Sb2Te3 film. With low temperature magnetometry, exchange bias is observed which is consistent with an exchange interaction between an antiferromagnet and an adjacent ferromagnet. Upon cross-section high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) of the interface between Sb2Te3 and Ni80Fe20 we observed a complex interface with diffusion and novel, secondary phase formation. The predominant phase at the interface was structurally consistent with a strained NiTe2-type phase. Density functional theory calculations revealed that the antiferromagnetism at the interface was due to the NiTe2-type structure with Fe in the Ni-site. This work emphasizes the chemical complexity of topological insulator/ferromagnet interfaces. These interfaces may host novel, metastable intrinsic magnetic topological phases and should be studied more in depth.15

9:45 AM

Synthesis and Design of Metal-Organic Framework Taggant Materials

Raphael Angelo Reyes*[1], Dorina Sava Gallis[1], Jacob Deneff[1], Eric Sikma[1]
1. Sandia National Labs

Polynuclear rare-earth metal-organic frameworks (REMOFs) are an emerging class of materials possessing tunable luminescent properties which can be applied as complex tag fluorophores.

In this study, we targeted a series of isostructural polynuclear REMOFs based on a tetratopic organic ligand (1,2,4,5 tetrakis(4-carboxyphenyl) benzene, TCPB) and nonanuclear metal clusters (M-TCPB, M=Eu, Gd, Yb). To probe the complex energy transfer mechanisms needed to efficiently control the resulting photoluminescent properties, we incorporated Eu (high-energy donor visible emitter), Yb (low-energy acceptor near-infrared emitter), and Gd (optically inactive) as a spacer to modulate energy transfer between Eu and Yb. A series of M-TCPB materials which included single, di, and trimetallic compositions were synthesized with varying metal ratios based on a ternary diagram. The structures of these materials were confirmed via powder X-ray diffraction and the metal distribution was probed via scanning electron microscopy/energy dispersive X-ray spectroscopy. Emission spectra and luminescent lifetimes photophysical characterization showed that by increasing the concentration of Yb in di- or trimetallic compositions, a decrease in lifetime is noted, with Gd effectively slowing down energy transfer between Eu and Yb.

This work demonstrates a versatile materials platform capable of multiplexed encoding in the time domain and amenable to authentication via tunable emission spectra and composition.

This work is supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories. 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-NA-0003525. SAND2022-12070 A.

10:00 AM

Optimizing Copper Deposition in High Aspect Ratio Through Silicon Vias

Jessica McDow*[1], Rebecca P. Schmitt[1], Mieko Hirabayashi[1], Jaime L. McClain[1], Matthew B. Jordan[1]
1. Sandia National Laboratories

We show an optimization method for filling high aspect ratio through silicon vias (TSVs) that provides insights into the diffusion and suppression kinetics of a superfilling electroplating chemistry. Full wafer thickness vias enable a TSV last processes applicable to split foundry models and/or can be used with large proof mass, microelectromechanical systems (MEMS). To electroplate full-wafer thickness TSVs, a suppressor only solution is required. The s-shaped negative differential resistance (S-NDR) bottom-up fill mechanism1,2 is sensitive to the via geometry and bath chemistry. A chemistry consisting of copper sulfate, sulfuric acid, potassium chloride, and Tetronic 701, we demonstrate a time-dependent process window where early on too high of an overpotential results in suppressor breakdown and too low of an overpotential results in complete suppression of the deposition process. Controlling the voltage between -520 mV (MSE) and -560 mV (MSE), we were able to demonstrate complete fill of the TSVs in 30% of the time previously required for filling. In this work, understanding of copper deposition kinetics in a suppressor only electrolyte and the development of optimized plating parameters utilizing the S-NDR mechanism is outlined.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2022-11995 A

1Rebecca P. Schmitt et al 2020 J. Electrochem. Soc. 167 162517.
2D. Josell and T. P. Moffat 2018 J. Electrochem. Soc. 165 D23.

10:15 AM

Interface trap state analysis of gate dielectrics on gallium nitride and silicon carbide using a modified C-ψ_S procedure

Brian Rummel*[1], Caleb Glaser[1], Luke Yates[1], Andrew Binder[1], Andrew Allerman[1], James Cooper[1], Robert Kaplar[1]
1. Sandia National Laboratories
2. Purdue University

The large breakdown electric field strength and high electron saturation velocity of wide band gap (WBG) materials make them favorable candidates for high-power and high-frequency applications. However, WBG-based structures exhibit large charge defect densities at or near the dielectric/semiconductor interfaces, introducing threshold-voltage instabilities in contemporary MOS devices. Furthermore, traditional capacitance-voltage (CV) techniques used to characterize the density of interface states for gate dielectrics, such as the high-low method, require unconventionally high probing frequencies to account for fast trap states associated with WBG materials.

The C-Ïˆ technique is a quasi-static CV characterization method known for determining interface trap distributions in WBG-MOS structures, such as MOS capacitors, and has been demonstrated for SiC-based systems. Nevertheless, the C-Ïˆ has been shown to be highly sensitive to systematic error and may lead to an incorrect evaluation of interface trap density distributions, especially in GaN-based systems. In this work, the C-Ïˆ method is successfully modified to accommodate both n-GaN and n-SiC systems and determines a closely bounded set of interface trap state density distributions constrained by reasonable mathematical conditions. This effort is part of a larger endeavor to fully capture the physics of WBG-MOS interfaces and reliably guide processing parameters to enhance device performance.

10:30 AM

Stable Radical Doping of Dielectric Films

Sarah Russell*[1] Jared Keever[2], Nathaniel A. Lynd[2], Alex Robinson[1], Leah Appelhans[1]
1. Sandia National Laboratories
2. The University of Texas at Austin, Austin, TX

Developing energy dense, lightweight polymer dielectrics would benefit aerospace, sensor, and solar cell industries where lighter, more efficient capacitors are desired. MylarÂ® film, biaxial-oriented polyethylene terephthalate, is widely used to manufacture capacitors. However, MylarÂ® has a relatively low energy density which limits capacitor and device build flexibility. In this work, we investigate the incorporation of small molecule stable radical species into commercial capacitor-grade Mylar film via solvent-based chemical doping. Our hypothesis is that these stable radical groups may increase energy density in two ways. First, they will increase the polarizability of the dielectric and, therefore, the permittivity. Second, and more importantly, they will act as deep electron traps, to increase breakdown strength. In prior work done by Feng et al., the stable radical species TEMPO (2,2,6,6-tetramethylpiperidine 1-oxyl), when blended with PMMA, was shown to improve energy density by 51% [1]. Inspired by this work, our goal is to develop a process for stable radical incorporation that will be adaptable to commercially available capacitor grade dielectric films. Various stable radical species are investigated for suitability as Mylar dopants. Stable radical concentration in films, experimental doping parameters, dielectric properties, and breakdown performance of stable radical-doped Mylar films are evaluated in this work.

[1] Y. Feng, T. S. Suga, H. Nishide, G. Chen and S. Li, "How to Install TEMPO in Dielectric Polymers - Their Rational Design toward Energy-Storable Materials," Macromolecular Rapid Communications, pp. 40, 1800734, 2019.

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10:45 AM
Break

Structural Materials and Failure Mechanisms

Room: Sandia Ballroom VII
Session Chair: Ashok Ghosh, New Mexico Tech

8:45 AM
Ductile failure - from the nanoscale conditions for void nucleation to the mechanisms of ductile rupture (Invited)

Philip Noell*[1], Julian E. C. Sabisch[1], Douglas L. Medlin[1], Jay D. Carroll[1], Brad L. Boyce[1]
1. Sandia National Laboratories
2. The University of Oklahoma

Ductile rupture often involves degradation of the structure from the nucleation and growth of voids and their coalescence into cracks. Current models of void nucleation at hard particles generally assume an elastic particle in a homogeneous, inelastic matrix. Fracture subsequently occurs when the stress at the particle/matrix interface exceeds the interfacial strength or fractures the particle. However, the critical microstructural conditions, such as dislocation boundaries and vacancy clusters, that enable these processes are poorly understood. To understand the role of these deformation-induced microstructural defects during void nucleation, the present study presents ex-situ cross-sectional observations of interrupted deformation experiments revealing incipient, subsurface voids in a copper material containing copper oxide inclusions. Subsequently, we present a summary of the mesoscale mechanisms by which voids grow and/or coalesce, ultimately leading to failure. In some cases, ductile failure can occur in the absence of voids.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

9:15 AM
Experiments and modeling of viscoelastic delamination through a transition in validity of small-scale-yielding

Brandon Clarke*[1], Rob Flicek[1], Dave Reedy[1], Todd Huber[1], Frank DelRio[1], Scott Grutzik[1]
1. Sandia National Laboratories

We present a set of interfacial fracture toughness data collected with asymmetric double-cantilever beam (ADCB) specimens consisting of aluminum adherends bonded with Epon 828/DEA epoxy. The ADCB specimens were tested over a range of quasistatic loading rates and temperatures between room temperature and just above the glass transition temperature of the epoxy adhesive. The results indicate a transition which we interpret as regimes where small-scale-yielding is either valid or invalid. In addition, we present efforts to predict the observed trends through finite element models which use a nonlinear viscoelastic material model to describe the epoxy behavior and cohesive surface elements to describe the interface separation.

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9:30 AM
Extreme SEM

Khalid Hattar*[1], Eric J. Lang[1]
1. Sandia National Laboratories

The Scanning Electron Microscope (SEM) has emerged as possibly the most ubiquitous characterization instrument in the field of materials science and has been used in the characterization of biomaterials through energy and structural materials to a range of advanced 3D printed materials. Sandia National Laboratories has developed an in-situ ion irradiation scanning electron microscope (I3SEM), which combines a field emission variable pressure scanning electron microscope, a 6 MV tandem accelerator, high flux low energy ion source, an 808 nm-wavelength laser, and multiple SEM stages to control the thermal and mechanical loading applied to the samples. This new facility advances real-time understanding of materials evolution under combined environments at the nanometer to millimeter length scales. This presentation will highlight several examples of possible in the overlapping extreme environments now possible, allowing for simultaneous ion irradiation, ion implantation, laser heating, conductive heating, cooling, and large range of mechanical deformation (nanoindentation, tensile loading, fatigue, creep, and many more conditions).

This work was performed at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

9:45 AM

Applications of Force Tensiometry for Characterizing Complex Materials Surfaces

Rachel Callaway*[1], J. Elliott Fowler[1]
1. Sandia National Laboratories

A material's surface often dictates its performance in critical engineering applications. Surfaces can be defined by characteristics such as topography, chemistry, and free surface energy; however, a single surface science tool is generally insensitive to at least one of these factors. For example, sessile contact angle goniometry is used to describe wettability; yet it is a static measurement and can't account for the role that topology plays. In addition, this method cannot be used to look at the wettability of unconventional surfaces such as powders. Force tensiometry is a technique that utilizes a microbalance to measure the mass changes as liquids interact with surfaces. Forces, as opposed to static angles, are descriptive of the dynamics taking place when a liquid, solid and gas interact at a surface. In this study, we show how adhesion measurements add additional information about surface roughness of various polymer coatings, where static contact angle goniometry was unable to resolve material differences. We also demonstrate how the water contact angle of MoS2 powders can be measured to discern differing amounts of contaminating hydrocarbons left over from the manufacturing process. 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-NA0003525. This talk describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the talk do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

10:00 AM

Characterization of Heterogeneity and Mechanical Properties of SiCf-SiCm Composites

James Nance*[1], Ghatu Subhash[1], Bhavani Sankar[1], Nam Ho Kim[1]
1. University of Flordia

Silicon carbide fiber-reinforced silicon carbide matrix composites (SiCf-SiCm) is a potential candidate material for high-temperature applications due to their excellent properties, such as high-temperature strength retention, high modulus, and strength, etc. Despite these promising characteristics, there is still a limited scope of understanding the performance and properties of these materials in the aforementioned applications. For example, there is an inherent heterogeneity that contributes to significant scatter in the strength and uncertainty of the composite. This presentation investigates automatic quantification techniques to measure this heterogeneity. Furthermore, the strength of the composites was evaluated under a variety of loading scenarios to determine which architectural features influence the strength the most.

10:15 AM

Elevated Temperature Behavior of Pinch Welded 304 and 316L Tube

Zahra Ghanbari*[1], T. Ivanoff[1], C. Laursen[1], D. Pendley[1], M. Maguire[1], C. Finfrock[1]
1. Sandia National Laboratories

Resistance pinch welding allows for sealing of tubing by applying simultaneous current and force to collapse a tube together and allow the interior walls to bond. For certain applications, pinch welded tubes are desired to survive elevated pressures during temperature excursions in excess of 1000 Â°C. These temperatures and pressures are near or beyond the available stress rupture literature data. Thus, elevated temperature pressure tests on resistance pinch welded 0.125â€□ outer diameter (nominally 0.030â€□ wall thickness) 304 and 316L stainless steel tubes were performed to understand weld survivability and general alloy performance. Both alloys exhibited good weld and tube performance via survival during multi-hour exposures at 1000 Â°C to pressures up to 1500 psi, and several minute exposures at pressures near 5000 psi. The pressurization was performed using nitrogen, and the effects of nitrogen uptake in the tube interior wall at high temperatures were also explored. The cracking behavior of the tubes and oxide development was characterized with multiple techniques, including light optical microscopy (LOM), scanning electron microscopy (SEM) and microhardness.

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10:30 AM

High Throughput Measurements of Coefficient of Thermal Expansion via Digital Image Correlation

Kaitlynn Conway*[1], Jay Carroll[1]
1. Sandia National Laboratories

Additive manufacturing is a highly manipulatable manufacturing process with many parameters from laser power to laser path that are adjustable for nearly infinite varying material property outputs. With such large property options, it is possible to rapidly print specimens with varying print parameters and material properties where a high throughput methodology to test various material properties is needed. Traditional coefficient of thermal expansion measurements involves heating a specimen and using a physical transducer to measure a specimen's change in length where the specimen moves the end of the transducer as it expands, limiting the test to one specimen as a time. A novel coefficient of thermal expansion measurement setup was developed to use digital image correlation as a non-contact method of measuring the expansion of the specimen allowing 50 specimens to be measured concurrently rapidly increasing the throughput of CTE measurements.

10:45 AM
Break

Biomaterials and Soft Materials

Room: Sandia Ballroom VII
Session Chair: Nathan Brady, Sandia National Laboratories

8:45 AM

Genetic Engineering for Bio-inorganic Materials

Kimberly Butler*[1]
1. Sandia National Laboratories

Biological systems synthesize complex bio-inorganic hybrid materials at the nano-, micro- and macroscale. These materials have unique properties including lightweight strong composites and self-healing and are synthesized using non-toxic and energy efficient methods. While all scales of bio-inorganic synthesis are of interest, advancements in macroscale biosynthesis lags the micro- and nanoscale due to the need to work in complex cellular systems. Genetic engineering provides a pathway to bioengineered bio-inorganics in complex cellular systems, and we will provide examples of two such systems here.

Living bone is a lightweight, heterogenous 3D structure able to withstand high impact and cyclic fatigue, moderate stress leads to improved strength, and the cells within bone are continuously sensing and repairing damage leading to optimized chemical composition for increased mechanical performance. Through chemical induction and engineering gene expression of different cells responsible for bone production and bone degradation, we have altered the remodeling potential in synthetic bone.

Mollusk nacre is one of the strongest natural materials due to the tiled subcomponents that interlock when stress is applied, spreading the strain to resist fracture. It is created via a 'brick-and-mortar' structure of nano-sized aragonite tablets glued together with organic material. In contrast to bone, where immortalized cells are available and the genetics well understood, mollusk engineering tools are nascent. We have developed protocols to obtain, culture and engineer mollusk mantle cells, laying the groundwork for genetically engineered nacre production.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:15 AM

The power of silica in nanomedicine and beyond

Achraf Noureddine*[1]
1. Department of Chemical and Biological Engineering, UNM

Silica science has been extensively exploited in various fields since the 19th century and has recently reached a new milestone by being approved by FDA as an investigational new drug development IND with the Cornell Dots imaging agent. Our UNM Nanoscience and Nanomedicine lab has longstanding experience in making and using silica-based nanotechnologies. The presentation will start by describing the evolutionary status of silica and related bioapplications, then will highlight our lab's recent discoveries including the use of CRISPR technology for gene editing, and delivery of nucleic acids for drug-resistant relapsed prostate cancer as well as small molecule inhibitors, chemotoxins or antiviral agents.

9:45 AM

Thermal Shock Effects on Phenolic Composite

Ryan Schoell*[1], Nathan Madden[1], Eun-Kyung Koss[1], LaRico Treadwell[1], Bernadette Hernandez-Sanchez[1], Khalid Hattar[1]
1. Sandia National Laboratories

The effect of heating rate on different phenolic composite materials was investigated in an in-situ transmission electron microscopy (TEM) study. Samples of phenolic composite matrix with silica fibers, carbon fibers, and no fibers were extracted with a focused ion beam to create TEM lamellas. Samples were either heated with a Gatan double tilt heating holder to a slow rate of 15 C/min or heated quickly with a 1064 nm 20 W infrared laser operating at 70% power for 10 ms. A slower laser heating was also conducted as a comparison. The effects of the heating rate on the microstructure were characterized in situ in the TEM, and the effects of the type of fiber were analyzed.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

10:00 AM

Mycosynthesis of Zinc Oxide Nanoparticles Exhibits Fungal Species Dependent Morphological Preference

Nathan Brady*[1]
1. Center for Integrated Nanotechnologies, Sandia National Laboratories

Filamentous fungi can synthesize a variety of nanoparticles (NPs), a process referred to as mycosynthesis that requires little energy input, does not require the use of harsh chemicals, occurs at near neutral pH, and does not produce toxic byproducts. While NP synthesis involves reaction between metal ions and exudates produced by the fungi, the chemical and biochemical parameters underlying this process remain poorly understood. Here, we investigated the role of fungal species and precursor salt on the mycosynthesis of zinc oxide (ZnO) NPs. Our data demonstrates that all five fungal species tested are able to produce ZnO structures that can be morphologically classified into (i) well-defined nanoparticles, (ii) coalesced/dissolving nanoparticles, and (iii) micron-sized square plates. Further, species dependent preferences for these morphologies were observed, suggesting potential differences in the profile or concentration of the biochemical constituents in their individual exudates. Our data also demonstrates that mycosynthesis of ZnO NPs was independent of the anion species, with nitrate, sulfate, and chloride showing no effect on NP production. These results enhance our understanding of factors controlling the mycosynthesis of ceramic NPs, supporting future studies that can enable control over the physical and chemical properties of NPs formed through this â€œgreenâ€ synthesis method

10:15 AM

High-Speed and High-Resolution 3D Printing of Self-healing and Ion-conductive Hydrogels via µCLIP

Wenbo Wang*[1], Xiangfan Chen[1]
1. School of Manufacturing Systems and Networks, Arizona State University

Ion-conductive self-healing (SH) hydrogels have received significant attention as biomaterials benefiting from the behavior of living tissue to broaden the design of health monitoring systems and soft robotics with autonomously SH capabilities. Herein, we propose a high-resolution 3D printing of ion-conductive SH hydrogel realized by micro-continuous liquid interface production (ÂµCLIP), which fully recovers the mechanical properties after 12h at room temperature without external trigger. These novel hydrogels are designed with interpenetrating polymer networks (IPN) based on physical-crosslinked poly(vinyl alcohol) networks combined with chemical/ionic crosslinked networks formed by acrylic acid and ferric chloride. In addition, the ionic conductivity and high stretchability of the hydrogel enables strain and pressure sensing capabilities that could be applied as health monitoring system or soft robotics. This novel approach of high-resolution 3D printing of SH hydrogels in complex structures will provide a promising development of future biomedical devices.

10:30 AM

Thermo-Rheometric Characterization of Nanolubricants for Space Applications

Ayten Bakhtiyarova*[1], Mostafa Hassanalian[1], Sayavur Bakhtiyarov[1]
1. New Mexico Institute of Mining and Technology
2. Mechanical Engineering Department

The conventional lubricating materials used in space have limited lifetimes in vacuum due to the catalytic degradation on metal surfaces, high vaporization at high temperatures, dewetting, and other disadvantages. The lubricants for the space applications must have specific properties such as vacuum stability, high viscosity index, low creep tendency, good elastohydrodynamic and boundary lubrication properties, optical or infrared transparency, and radiation atomic oxygen resistance. The addition of nanoparticles is one of the methods to enhance the thermophysical and heat transfer properties of liquid lubricants. Some of these properties for liquid lubricants are volatility, creep, surface tension, viscosity, chemical composition, weight loss, density, vapor pressure, etc. The rheological and heat and mass transfer measurements for newly developed two nanolubricants were measured experimentally using Differential Scanning Calorimetry (DSC), rotational rheometer of â€œparallel-platesâ€ mode and Thermogravimetric Analyzer (TGA).

10:45 AM

Break

Kreidal Memorial Lecture

Room: Sandia Ballroom

11:00 AM

Analysis and Simulation Guided Process and Properties of Anisotropic Hierarchical Porous Ceramics for Energy Conversion and Storage

Rajendra K. Bordia*[1]
1. Materials Science and Engineering, Clemson University

Ion-conductive self-healing Our current research is focused on developing processing strategies to control the microstructure of ceramics at different length scales. One of the focal areas porous ceramics produced by controlled sintering of powder compacts. Many of the applications of porous ceramics demand optimization of a multitude of properties some of which have conflicting requirements on the microstructure. Materials with designed anisotropic and/or hierarchical microstructures have the potential to optimally address the requirements.

We will first present a broad overview of the use of porous ceramics in advanced energy conversion and storage applications including the property requirements. Next, we will present results from our collaborative projects focused on microstructural control in hierarchical and/or anisotropic porous ceramics. Porous ceramics are used in a broad range of technologies of interest to energy conversion and storage including electrochemical applications like electrodes for solid oxide fuel cells, high temperature insulators, thermal energy storage and electrochemical energy storage. In these applications, a multitude of properties are of interest. For specific applications, a subset of mechanical, thermal, electrical and ionic conductivity, gas diffusion and chemical reactivity need to be optimized. In this presentation, results will be presented on the processing approaches to make these designed microstructures, the quantification of the 3D microstructure at different length scales and simulations to design optimal microstructures for specific applications including electrodes for solid oxide fuel cells and electrolysis cells, and Li-ion batteries

The research in the is supported by the US National Science Foundation

12:00 PM

Lunch (Provided)

Theory and Modeling

Room: Piñon

Session Chair: Brian Lester, Sandia National Labs

1:00 PM

Determination of FDTR Lateral Resolution for Heterogeneously Integrated Micro Electronics

Brenden Herkenhoff*[1], Wyatt Hodges[1], Benjamin Treweek[1], Amun Jarzembski[1], Timothy Walsh[1], Gregory Pickrell[1]

1. Sandia National Labs
2. New Mexico Institute of Mining and Technology

With the advancement of microelectronic manufacturing in recent years, new technologies must be developed to provide quality assurance and improve device reliability for the proliferation of Heterogeneously Integrated (HI) electronics. It is therefore critical to develop highly precise diagnostics to better understand the behavior of HI systems under various use and aging conditions, with particular emphasis on testing interconnect integrity. Thermal property measurement techniques, such as Frequency Domain Thermoreflectance (FDTR), offer a potential solution by determining bond integrity through the measurement of interfacial thermal properties between a metal interconnect and chiplet. This technique provides a nondestructive evaluation method by non-contact optical pump and probe lasers in which the changes in surface reflectance due to thermal variations can be measured. This work aims to model the limits of this technique to determine the lateral resolutions the FDTR technique can provide at various depths. This work focuses on the variation of geometric model parameters and the use of a finite element analysis model to provide insight into the limits of FDTR for diagnostics in HI systems. The model under investigation consists of the gold transducer layer, a silicon layer representing a chiplet, followed by a contact resistance, metal interconnects and a silicon chiplet backside. Interconnect size, interconnect periodicity, device thickness, and interconnect thickness will be explored. The variation in model geometry allows for future comparison with experimental data to determine the health of interconnects through nondestructive testing and evaluation with a noncontact method.

1:15 PM

Modeling the Stability of FePc-Functionalized Graphene and Enhanced ORR Activity of Ligand Exchanges and Substrate Variations

Naomi Helsel*[1], Pabitra Choudhury[1]

1. Chemical Engineering Department, New Mexico Institute of Mining of Technology

Finding a platinum-free cathode catalyst that effectively model the oxygen reduction reaction (ORR) of a proton-exchange membrane (PEM) fuel cell cathode better than the current commercial Pt/C catalyst has been a major shortcoming in fuel cell technology. Overall, a promising platinum-free cathode catalyst must offer great ORR activity, ORR selectivity, and acid stability. This work analyzes the stability and tuning of a potential Pt-free fuel cell catalyst, an iron phthalocyanine monolayer supported on a graphene substrate (GFePc). GFePc has been studied previously through density functional theory (DFT) calculations for its enticing ORR activity and selectivity to the preferred four-electron ORR pathway. Utilizing ab inito spin-polarized DFT calculations, the dominating pathway of the oxygen reduction (ORR) has been simulated along with defining its rate-limiting step to quantify ORR overpotential (indicator of catalyst reactivity/performance). Tuning GFePc via the ligand exchange of FePc, substate doping, and defect incorporation into the graphene substrate can offer enhanced ORR activity. We also tested tetra-substituted phthalocyanines (carboxy-, nitro-, and amino-) and hexadeca-substituted phthalocyanines (chloro-, fluoro-, and amino-) to check the effect of ligand exchange on the ORR activity. Overall, the DFT results show that ~1 at. % boron doping in conjunction with a mono-vacancy graphene substrate offers the best performance in both ORR and OER reactions. The stability of both GFePc and boron-doped GFePc (BGFePc) were also quantitatively modeled through the possible dissolution reactions via various intermediates during the ORR to computationally determine catalysts' stability as a function of potential and pH. The results also show that BGFePc, the structure in which boron-doped graphene is introduced, offers higher stability than the pristine GFePc structure in the potential and pH regions at which rotating disk electrode (RDE) experiments and PEM fuel cell operations would normally take place. The present study that allows for expanded understanding of the stability of GFePc, activity of substituted GFePc, and the effects that the tested substituents have on GFePc's performance as a cathode single-metal-atom based fuel cell catalyst will also be discussed.

Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support (or partial support) of this research. The work is supported by ACS-PRF Grant No [58740-UR6]. This work used the Extreme Science and Engineering Discovery Environment (XSEDE) TACC at the stampede2 through allocation [TGDMR140131]. This work utilized resources from the University of Colorado Boulder Research Computing Group, which is supported by the National Science Foundation (awards ACI-1532235 and ACI-1532236), the University of Colorado Boulder, and Colorado. PCC Cluster, NM Consortium, NM.

1:30 PM

Silicon Heterojunction solar cell device optimization using TCAD simulations and machine learning models

Rahul Jaiswal*, Tito Busani
1. Center of High Technology Materials – Albuquerque
2. University of New Mexico - Electrical & Computer Engineering

Solar cells are optoelectronic semiconductor devices, and solar cell technology is defined by its material and design parameters, depending on these parameters, the cell will perform with a certain performance metric set. The device architecture and its fabrication recipes are being continuously optimized but conventionally manufacturers have been trying to perfect their recipe using a hit & trial approach where multiple experiments are done to evaluate the best process conditions and device parameters, these strategies are resource & time expensive. In the past couple of decades simulation techniques are also being utilized in addition to the conventional approaches and very recently use of data science-based techniques has become popular in research and is gaining some traction in the PV industry.

The fundamental goal of this project is to provide a software interface which can predict cell performance metrics like its efficiency given a particular set of design and material parameters as input. Internally this interface will contain a trained machine learning model. The end user can be a researcher, a process engineer or even an automated machine like a robotic arm sorting good cells from bad cells.

This project starts by first designing a TCAD based device simulation model for simulating the electrical and optical properties of a solar cell, then this simulation model is calibrated to the performance of an industrially manufactured solar cell (Using characterization data), this calibration is assisted by statistical models. Finally, data from the calibrated simulations are used to train a machine learning model that acts as a digital twin for the physical device. Using these prediction modelling approaches newer device prototypes can be conceptualized with resources that are exponentially less compared to that required when using conventional approaches. The device targeted for this presentation is the silicon heterojunction solar cell or Heterojunction with thin intrinsic layer solar cell.

1:45 PM

Extracting Anisotropy Strength and Interfacial Free Energy of Al-Mg Alloy Using Molecular Dynamics Simulations

Daniel Dolce*[1], Amrutdyuti Swamy[1], Jeffrey Hoyt[1], Pabitra Choudhury[1]
1. Chemical Engineering Dept, New Mexico Institute of Mining and Technology, Socorro, NM 87801 USA
2. Materials Engineering Dept, New Mexico Institute of Mining and Technology, Socorro, NM 87801 USA
3. Materials Science and Engineering Dept, McMaster University, Hamilton, ON, Canada

The solidification microstructures of metals and alloys are strongly affected by solid-liquid interfacial properties. The anisotropy of the interfacial free energy (Î³) has an especially strong impact on both the tip radius and growth direction of dendrite microstructures. The Al-Mg binary alloy was studied at various undercooling temperatures to determine if a possible temperature dependence of the anisotropy of Î³ exists. The Capillary Fluctuation Method (CFM) is widely used due to its ability relate the anisotropy to the interfacial stiffness (S), which is an easier parameter to both simulate and measure. Equilibrium atomic simulations were performed using Molecular Dynamics (MD) in the Large-Scale-Atomic/Molecular Massively Parallel Simulator (LAMMPS) using a Modified Embedded Atom Method (MEAM) interatomic potential from the NIST IPR database. The solid-liquid interface was identified using an order parameter for the (100) and (110) orientations at undercooling temperatures of 910, 850, and 750K and the anisotropic parameters Îµ1 and Îµ2 were determined. It was found that the interfacial free energy typically followed a relationship of Î³100 > Î³110 > Î³111. Except for 910K which followed a Î³110 > Î³100 > Î³111 relationship. Superimposition of Îµ1 and Îµ2 on the already established orientation selection map predicts dendrite growth in the (100) direction at 910K followed by a switch to a hyperbranched direction at 850K, followed by a return to the (100) direction at 750K.

2:00 PM

Extracting Solid-Melt Interfacial Free Energy and Anisotropy Strength of Al-Cu Alloy Using Molecular Dynamics Simulations

Amrutdyuti Swamy*[1]
1. New Mexico Institute of Mining & Technology

Laser Melt Deposition is one of the growing additive manufacturing techniques employed in industries for creating new and improved materials. During this process, rapid solidification of the melt has been known to form cracks for an Al-Cu system. These cracks impede the overall strength of the material. Understanding the changes in interfacial free energy can help throw light on crystal growth & crack propagation during these rapid solidification operations. We have tried to analyze the role of undercooling and solute composition on interfacial free energy for an Al-Cu system using molecular dynamics and the capillary fluctuation method. An Al-Cu phase diagram was first generated for the interatomic potential in use. Crystal-melt interfaces were then created for different undercooling regimes using molecular dynamics, equipped with the solute composition information from the phase diagram. The equilibrium crystal-melt interfaces are then analyzed using the capillary fluctuation method to obtain the interfacial free energy and its anisotropy parameters. Our results show that the interfacial energy for the binary Al-Cu system does not have a linear dependence with solute composition or the amount of undercooling. The results also correctly predict the transition of dendrite growth orientations from (100) to (110) with Cu doping.

Acknowledgments: The work is supported by ARL Grant No. W911NF-2020032 and used the Extreme Science and Engineering Discovery Environment (XSEDE) TACC at the stampede2 through allocation [TGDMR140131]. This work utilized resources from the University of Colorado Boulder Research Computing Group, which is supported by the National Science Foundation (awards ACI-1532235 and ACI-1532236), the University of Colorado Boulder, and Colorado.

2:15 PM
Break

Session Chair: Stanley Chou, Sandia National Labs

2:30 PM
Phase Field Simulation of Aluminum Alloy solidification

Atiqur Rahman*[1]
1. New Mexico Institute of Mining & Technology

The microstructure formed during the solidification process controls the end properties of the most engineered materials. Understanding the formation of microstructure will provide the underlying physical mechanism of the solidification process and help to predict microstructure shape without needing an experiment that will give the advantage of manufacturing alloys with desired properties. While tracking moving interfaces is exceedingly computationally demanding, the Phase-Field model has demonstrated its effectiveness in simulating microstructure development processes without the need to explicitly track complicated interface dynamics. This research studied the effects of concentration, undercooling rate, and anisotropy on the morphology of dendrites. A phase-field model for the dendritic development of an Al-based binary alloy was simulated in this study. The overall findings from the solidification model indicate that increasing solute concentration delays solute rejection at the interface until a critical point. At a greater undercooling rate, dendrites grow into a more developed form, and the length of the principal dendritic arm expands with anisotropic effects.

2:45 PM
Thermodynamic properties of body-centered-cubic (BCC) refractory, BCC, high-entropy alloys: NbTaTiV, TaNbHfZrTi, VNbMoTaW

Danielsen Moreno*[1], Chelsey Hargather[1]
1. New Mexico Institute of Mining and Technology

BCC refractory high-entropy alloys (HEAs) are potential candidates for high-performance engineering material applications. At high temperatures, these HEAs show potential to outperform traditional nickel-based superalloys. By implementing first principles, ab initio calculations based on Density Functional Theory (DFT), thermodynamic and elastic properties were investigated. In this study thermodynamic properties such as entropy, enthalpy, heat capacity, and thermal expansion are presented. The BCC refractory HEAs in this study are NbTaTiV, TaNbHfZrTi, and VNbMoTaW. The results are compared to experimental values for validation.

Low Dimension / 2D Materials

Room: Piñon
Session Chair: Stanley Chou, Sandia National Labs

3:00 PM
Two-dimensional Silicon Carbide: An Emerging Semiconducting Material (Invited)

Sakineh Chabi*[1]
1. University of New Mexico

In the past decade, research in the field of two-dimensional materials has exponentially transitioned from fundamental studies to the development of complex 2D devices. While an increasing number of 2D materials have been synthesized successfully in the lab, others have only been theoretically predicted. One very important example is two-dimensional silicon carbide (2D SiC). Theoretical studies have predicted that monolayer SiC has a stable planar graphene-like honeycomb structure, a direct wide bandgap of about 2.58 eV, strong excitonic effects, and highly tunable electronic, optical, and magnetic properties. Further, one of the biggest advantages of 2D SiC over any other 2D material is its high-temperature capabilities. These characteristics are critical for many applications and make 2D SiC a potential game-changer for future energy-related technologies. Experimentally, however, the growth of 2D SiC has challenged scientists for decades.

Importantly though, our group has made ground-breaking progress on the synthesis of 2D SiC and bridged the gap between theory and experiment. In my talk, I will discuss our latest progress on 2D SiC and related material.

3:30 PM
GROWTH AND DRY TRANSFER OF GRAPHENE ON SAPPHIRE

Kenneth Liechti*[1], Sivasakthya Mohan[1], Deji Akinwande[1]
1. University of Texas Austin

Mechanical delamination of graphene from its growth substrate is an effective, clean, dry transfer method that overcomes the disadvantages of traditional wet transfer approaches such as long processing times, polymeric residues, and harsh chemical exposure of the transferred films . However, it is challenging to use copper foil, which is a widely used growth substrate, in the transfer process due to its lack of mechanical rigidity. Thin copper films deposited on silicon wafers have been used to overcome this difficulty. However, a very high initial thickness of copper film (~ 1Î¼m) needs to be deposited to avoid dewetting problems that occur during the high temperature growth on copper films. To this end, we have studied the metal-free synthesis of graphene on sapphire substrates, which has been shown in literature to have a sufficiently low adhesion energy with graphene.

In this work, we have performed atmospheric pressure chemical vapor deposition to grow graphene on sapphire. The as-grown graphene was characterized using Raman spectroscopy, scanning electron microscopy (SEM), atomic force microscopy (AFM) and X-ray photoelectron spectroscopy. Prior to growth the sapphire substrates were annealed in air at high temperatures to achieve a suitable surface reconstruction of the sapphire surface needed to grow high quality graphene. The annealing has helped decrease the density of wrinkles of graphene on sapphire and caused a reduction in the D/G Raman peak ratio of the graphene. With annealing we have achieved a D/G ratio as low as 0.19 for the graphene grown at 1050ËšC, which is among the lowest reported values in literature, thus proving the graphene to be of high quality. Graphene based transistors were fabricated from the as-grown films and electrical characterization was done to extract mobility.

Furthermore mode I fracture experiments have been conducted on double cantilever beam type sandwich specimens of sapphire/graphene/epoxy/sapphire, using a dual actuator loading device, to obtain the mode I toughness and traction-separation relation of the interface between graphene and sapphire. The high quality of the transferred films was confirmed by Raman mapping, SEM and AFM and electrical characterization.

3:45 PM

Engineering of Nanoscale Heterogenous Transition Metal Dichalcogenide-Au Interfaces

Alex Boehm*[1], Jose J. Fonseca[1], Konrad Thürmer[1], Joshua D. Sugar[1], Catalin D. Spataru[1], Jeremy T. Robinson[1], Taisuke Ohta[1],
1. Sandia National Laboratories, Albuquerque, NM
2. Sandia National Laboratories, Livermore, CA
3. Jacobs Technology Contractor at the U.S. Naval Research Laboratory, Washington, DC
4. US Naval Research Laboratory, Washington, DC

Transition metal dichalcogenides (TMDs) have garnered much attention owing to their extraordinary chemical, electrical, and optical properties. However, early material studies have revealed that these properties can be greatly impacted by extrinsic factors and thus a careful understanding of how TMDs interface with other materials is crucial. Particularly in the case of metallic contacts, where the Schottky barrier height (SBH) is a key parameter for determining contact resistance and maximum device performance. The archetypal method for extracting SBH from transport measurements average over the entire contact area. This neglects local variations or heterogeneities which can result in â€˜hot' and â€˜cold' spots for charge transfer that could limit device performance. Recent reports have revealed spatial nonuniformities in contact resistance and interaction strength at MoS2â€“Au interfaces. In this work, by directly probing the electronic structures of WS2â€“Au and WSe2â€“Au interfaces with high spatial resolution, we delineate nanoscale heterogeneities in the composite systems that give rise to local variation in electronic structure and SBH across the interface. Spectroscopic analysis reveals key differences in TMD work function and binding energies for the occupied electronic states (>100 meV) that we correlate with differing crystallite orientations in the Au contact, suggesting an inherent role of metal microstructure in contact formation. We then leverage our understanding to develop processing techniques to form homogenous TMD-Au interfaces. These insights are relevant for any device applications involving metal contacts with TMDs and emphasize that the microstructure of contacts deserves close consideration.

Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, 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-NA-0003525.

Electronics, Magnetics and Photonic Materials & Devices

Room: Sandia Ballroom VI
Session Chair: Eric Lang, University of New Mexico

1:00 PM

Lattice multipole resonances in periodic nanostructures and metasurfaces

Md Sakibul Islam*[1], Viktoriia Babicheva[1]
1. Department of Electrical and Computer Engineering, University of New Mexico

Arranging nanoparticles into a periodic array can induced drastic changes in the metastructure resonances. Periodic nanoparticle arrays give rise to lattice resonances at the wavelength close to the Rayleigh anomaly, i.e., effective wavelength in the medium is equal to the array period. This often facilitates the excitation of additional resonances known as lattice resonances.

In this work, we aim to design efficient directional scatterers and their arrays for metasurfaces and transdimensional metastructures. The combination of different materials in the nanoparticle allows the tune of electric and magnetic resonances of the nanoparticles and achieving broadband overlap. The nanofabrication and characterization include sample preparation, deposition of metals and oxides, as well as optical measurements of reflection and transmission spectra. One or multiple nanoparticles (or scattering elements, or scatterers) are considered in the unit cell of the lattice unit. We introduce mismatched resonances excited in the array and show that the dimensions of scatterers define the type and character of excitations.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy

(DOE) Office of Science by Los Alamos National Laboratory (Contract 89233218CNA000001) and Sandia National Laboratories (Contract DE-NA-0003525).

1:15 PM

Controlling Interface Interactions in Granular Metal Thin Films

Simeon Gilbert*[1], Melissa Meyerson[1], Samantha Rosenberg[1], Paul Kotula[1], Nathan Madden[1], Peter A. Sharma[1], Jack Flicker[1], Michael Siegal[1], Laura Biedermann[1],
1. Sandia National Laboratories

Granular metals (GMs) are composed of nanoscale metal islands surrounded by an insulator. At volumetric metal fractions (Ï†) below the percolation threshold (Ï†c), GMs are insulating, and for Ï†>Ï†c they are metallic. Au- and Ag-based GMs exhibit a sharp conductivity (Ïƒ) knee at Ï†c, with Ïƒ increasing 4-6 orders-of-magnitude with Î”Ï†â‰ˆ0.1. However, most other GMs utilize non-noble metals paired with an oxide insulator and exhibit 1-3 orders-of-magnitude Ïƒ changes at Ï†c. We have found that this reduced change in Ïƒ at Ï†c is due to deleterious metal-insulator interface states as indicated by x-ray photoemission spectroscopy. The change in Ïƒ at Ï†c can be increased by choosing appropriate metal-insulator combinations and deposition conditions. For example, when our Mo-SiNx GMs are sputtered in an Ar/H/N environment, rather than pure Ar, Ïƒ is reduced by 3-4 orders-of-magnitude for Ï†<Ï†c. Additionally, the interface effects can be mitigated by increasing the separation distance between metal islands via post-growth annealing which can result in >6 orders-of-magnitude decreases in Ïƒ when Ï†<Ï†c. Future work will further explore manipulating the island morphology and interface interactions in order to tune the conductivity mechanisms in GMs.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories (SNL). SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Energy Nuclear Materials

Room: Sandia Ballroom VI
Session Chair: Eric Lang, University of New Mexico

1:30 PM

Process Development of Ferritic Steels for High Dose Fast Reactor Applications (Invited)

Stuart Maloy*[1], M. Toloczko[1], C. Lavender[1], B. Eftink[2], T.A. Saleh[2], T.J. Lienert[3], G.R. Odette[4], T.S. Byun[5], J. DeCarlan[6], D. Sornin[6]
1. Pacific Northwest National Laboratory
2. Los Alamos National Laboratory
3. Optomec Corporation, Albuquerque, NM 87109,
5. University of California, Santa Barbara
6. Oak Ridge National Laboratory

The Nuclear Technology R&D program has significant experience at qualifying metallic fuels for fast reactor applications. In this process, new fuels and cladding materials must be developed and tested to high burnup levels (e.g. >20%) requiring cladding to withstand very high doses (greater than 200 dpa) while in contact with the coolant and the fuel. Previous research has been performed on tempered martensitic steels such as HT9 to doses up to 155 dpa. In addition, new ferritic/martensitic and ferritic Oxide Dispersion Strengthened (ODS) alloys are being developed with improved radiation tolerance. In recent research, ferritic/martensitic steels have been produced using additive manufacturing showing similar properties to wrought materials after normalizing and tempering the microstructure. Also, in the as-deposited condition, additively manufactured grade 91 steel shows a significant increase in yield strength at 300 Â°C and 600Â°C over that measured for wrought normalized and tempered material. In addition, ferritic ODS alloys are being processed into tube form and tested for future nuclear applications. Tubes over 3 feet in length are being produced by pilger processing. Recent progress in high dose irradiated materials testing and materials development will be presented.

2:00 PM

Current and future advances in plasma-facing materials to enable nuclear fusion

Eric Lang*[1], Khalid Hattar[1]
1. University of New Mexico
2. Sandia National Laboratories

The plasma-material interface in nuclear fusion reactors represents one of the harshest environmental service conditions for materials, exposing them to 14 MeV neutron bombardment, low energy deuterium (D) and helium (He) bombardment, steady state temperatures above 400°C and transient heat fluxes >1GW/m2. Currently, tungsten (W) is proposed as the plasma-facing material of choice for its high-Z nature, high melting point, and low H retention properties. However, W is inherently brittle, is further embrittled under irradiation, and develops undesired surface nanostructures under He irradiation. Numerous strategies have been employed to improve the performance of W in a fusion reactor setting. This talk will highlight developments in tungsten, including nanocrystalline W, dispersion-strengthened W, refractory complex concentrated alloys, and additively manufactured refractory alloys. This work will focus on experimental advances in understanding of material evolution in the extreme nuclear fusion reactor environment, especially in the realm of in situ experimentation and characterization of materials under He irradiation, high temperatures (>800°C), and mechanical stress. This work will highlight the advances of W regarding He management, microstructure stabilization, and advanced manufacturing and discuss further challenges and experiments needed to design and qualify advanced materials for use in a fusion environment.

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2:15 PM
Break

Session Chair: James Nance, Sandia National Labs
2:30 PM
Radiation Damage in Nuclear Materials: Helium Effects (Invited)
Y.Q. Wang*[1]
1. Los Alamos National Laboratory

Fast neutron interactions with materials produce not only atomic displacement damage but also incorporate helium atoms in lattice structure through nuclear reactions. Despite its chemical benignity, the small size of a helium atom combined with its near insolubility in almost every solid makes the heliumâ€"solid interaction extremely complex over multiple length and time scales. As a result, helium effects on microstructure evolution and thermo-mechanical properties can have a significant impact on the operation and lifetime of many applications, including advanced structural steels in fast fission reactors, plasma facing and structural materials in fusion devices, spallation neutron target designs, energetic alpha emissions in actinides, helium precipitation in tritium-containing materials, and nuclear waste materials.

3:00 PM
Electrolyte Design for Stable Multivalent Metal Anodes
Scott McClary*[1], Daniel Long[1], Kathryn Small[1], Alan Landers[1], Ana Sanz-Matias[1], Paul Kotula[1], David Prendergast[1]
1. Sandia National Laboratories
2. Lawrence Berkeley National Laboratory
3. Joint Center for Energy Storage Research (JCESR)

Multivalent (MV) metal (e.g. Ca or Mg) anodes are attractive for rechargeable batteries due to these materials' high capacities, abundant reserves, and low reduction potentials. However, developing commercially viable MV batteries is challenging because anodes are often passivated by electrolyte decomposition products, suppressing charge transport in subsequent cycles. Efficient MV batteries require a solid electrolyte interphase (SEI) that permits cation percolation while sufficiently blocking electron transport.

This work establishes design principles for MV electrolytes through multimodal characterization of a best-in-class Ca SEI. The principal technique we use is cryogenic transmission electron microscopy, which enables characterization of the air-sensitive SEI in its unperturbed state. We show that a thin nanocrystalline calcium oxide with minor calcium borate and carbonate fractions forms an effective SEI for Ca cycling [1]. Density functional theory calculations demonstrate that unique interfacial speciation is critical in forming this heterogeneous SEI. We alter Ca2+ speciation by introducing a second salt to the electrolyte, which modifies the SEI and electrochemical response. Our results establish direct correlations between electrolyte speciation, SEI chemistry and structure, and electrochemical performance. Such critical insight can inform the design of practical electrolytes and SEIs for rechargeable multivalent batteries.

[1] McClary et al. ACS Energy Letters 2022, 7(8), 2792-2800.

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3:15 PM
Diffusion-mitigated preservation of Mn and void swelling response under heavy ion irradiation at high temperature
Calvin Parkin*[1], Michael Moorehead[1], Lingfeng He[1], Kumar Sridharan[1], Khalid Hattar[1], Adrien Couet[1]
1. Sandia National Laboratories
2. University of Wisconsin- Madison
3. Idaho National Laboratory
This talk aims to provide a brief update on state-of-the-art irradiation materials research capabilities to study helium effects as well as on advanced materials design concepts in mitigating helium impact on thermomechanical properties of materials in radiation extreme conditions.

3:30 PM
Improved Electrostatic Modeling of Wind-Turbine Lightning Receptors and Evaluation of Novel Designs
Sidharth Arun kumar*[1], Ashok K Ghosh[1], Richard Sonnenfeld[1], Yeqing Wang[1]
1. New Mexico Tech
2. New Mexico Tech
3. New Mexico Tech
4. University of Florida

Due to scarcity of fast neutron irradiation capabilities as well as unwanted yet unavoidable activation, dual ion beam irradiation, concurrently from a heavy ion beam and a helium ion beam, has been used to study separate or synergistic effects of cascade damage and/or helium impact on materials microstructure, and thus to help establish scientific foundations for development of new concepts for improving the properties of existing alloys or designing new materials with exceptional radiation resistance.

3:45 PM
Ceramic/Metal Hybrid Membranes for High Temperature H2 Separation
Isabel Ibarra*[1], Ian Alsobrook[1]
1. CBE, UNM
2. CMEM, UNM
3. DOB, UNM

4. CISTAR

The recent oil price shock highlights the importance of a more efficient transformation of hydrocarbon resources into added-value chemical and fuel products, all while maintaining low environmental impacts. A well-studied method for olefin synthesis is C2-C5 alkane dehydrogenation. The hydrocarbons come from natural gas from fracking which is an abundant source. Catalytic dehydrogenation is limited by thermodynamic equilibrium conversions due to the reversibility of dehydrogenation reactions. Our goal is to develop a thermally stable, high flux membrane for selective removal of H2, a dehydrogenation product, which promotes the forward reaction. Once H2 removal is successful, we can expect to be able to dehydrogenate hydrocarbons at lower temperatures and increase the lifetime and stability of catalysts. Our ultra-thin membrane is prepared on porous anodic alumina via spin coating followed by three successive aging conditions that promote evaporation-induced self-assembly. Following calcination, the membrane is prepped for Pd or dense SiO2 ALD by a passivation treatment with HMDS and a partial reactivation via O2 plasma. An etching technique was developed for the extraction of the silica nanotubes. The nanotubes are electron transparent enabling direct TEM imaging of Pd or dense silica using UNM's high-resolution JEOL NeoARM TEM. The membrane's performance is determined by testing in a high-temperature mixed-gas permeation apparatus and permeate analysis via gas chromatography. Previous results demonstrated 1000 Barrer permeability with significant H2/Methane selectivity at 800Â°C.

Structural Materials and Failure Mechanisms

Room: Sandia Ballroom VII
Session Chair: Zahra Ghanbari

1:00 PM

Comparative investigation of high temperature behavior of uncoated and aluminum coated DADI substrates (Invited)

Olga Tsurtsumia*[1], Lili Nadaraia[1], Elguja Kutelia[1], Tengiz Kukava[1], Bronislava Gorr[2], Sayavur Bakhtiyarov[3]
1. Georgian Technical University
2. Karlsruhe Institute of Technology (Germany)
3. New Mexico Institute of Mining and Technology (USA)

To increase the efficiency of power plants it is necessary to rise their operating temperatures. This will cause placing a greater physical, chemical and mechanical demands on the materials applied. Hence, modernization and improvement of existing or development of novel materials is greatly needed. With this motivation in mind, advancement of high temperature oxidation properties of Deformable Austempered Ductile Iron (DADI, composed of: C â€“ 3.7, Si â€“ 1.0, Mn â€“ 0.3, Al â€“ 1.8, Mg â€“ 0.04 wt % in a Fe bulk) was successfully performed with the application of Al slurry coatings. For the comparison reasons the uncoated specimens of DADI were studied together with the aluminized ones. To achieve the best oxidation performance of the aluminized DADI specimens, first, three different microalloyed compositions of the uncoated material went through various thermal pretreatment schemes of austempering during their metallurgical preparation. They were carefully studied from the structural and phase composition viewpoints, and their properties at the elevated temperatures were evaluated. As a result, the most promising composition of DADI and an appropriate heat treatment scheme has been determined and further applied for the specimens to be slurry coated. The oxidation experiments ran at 650Â°C in air for 100 hours to study the high temperature kinetics as well as the structural peculiarities of the developed oxide scales. Drastically improved oxidation resistance was observed for the slurry aluminized specimens compared with uncoated ones. The weight gain reduction was achieved at the elevated temperatures by the factor of seven for the aluminized DADIs ensured by the spinel formation (mainly FeAl2O4) while uncoated specimens formed the poorly protective pure iron oxide and it was much thicker and less dense.

Acknowledgment: This work was supported by Shota Rustaveli National Science foundation of Georgia (SRNSFG) grant number FR-21-869.

1:30 PM

The Influence of Dimensional Deviations on the Performance of Welded 316 and 17-4 Stainless Steels

Mark Foster*[1]
1. Sandia National Laboratories

Welded joints from structures to components are used throughout many industries. Despite their ubiquity in application, welds can exhibit multiple geometric nonconformances affecting their overall performance. Past efforts have characterized bulk performance of welds in stainless steels, with many focusing on the effects of joining methodologies. Here localized weld dimensions in various gas tungsten arc welded (GTAW) and laser welded 316L and 17-4 stainless steels were examined using statistical techniques to determine their individual and combined influence on overall weld performance. Penetration depth and porosity were seen to be primary contributors to weld ultimate load.

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1:45 PM

Development of a high-temperature and high-pressure electrical feedthrough

Edward Arata*[1], Chowdary Koripella[1]
1. Sandia National Laboratories, Albuquerque, NM 87185, USA

Small sized electrical feedthroughs typically cannot survive exposure to air at high temperatures and pressures. Here we discuss the design aspects of feedthrough designed to survive 1000Â°C and greater than 1000 psi. Feasibility studies were performed by working through external vendors on a few selected designs with appropriate material choices to fabricate prototypes for evaluations. High temperature oxidizing

atmosphere exposure tests at ambient atmospheric pressure and at high pressures were performed. Leak tests and microstructure characterization were performed to understand the design weaknesses and to guide future designs for the development of a robust high temperature and high-pressure compatible feedthrough.

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2:00 PM

Underwater High Frequency Characteristics of Fluid-Filled Cellular Composites

Ashok Ghosh*[1]
1. Mechanical Engineering , New Mexico Tech, Socorro 87801

Fluid-Filled Cellular Composite (FFCC) is a biomimetic material with multiple functions. Inspired by the design of human skull, the FFCC is has a sandwiched construction of skin layers surrounding a fluid-filled porous composite core. This unique structure provides potential for multiple applications including in mechanical system, for impact resistance, acoustic damping, thermal management, and radiation shielding. This paper will discuss underwater high frequency characteristics of FFCC panels.

Wide range of tests were performed to characterize FFCC panels under acoustics environment, low and high frequency in air and in underwater high frequency to determine their Stealth Characteristics. Within the frequency range of 250-1000 Hz, the material was found to have 25% higher acoustic transmission loss (TL) than that predicted by the acoustic mass law. As high as 132dB transmission loss (TL) through a Â½ inch thick sample was noticed. Influence of fluid in the pores was found to be around 36 dB, equivalent to a layer of 5â€□ building wall with 2â€□x 4â€□ stud framing covered by 2 sheets of gypsum board on both sides.

Variations in density, temperature, pressure and underwater salinity all can influence the behavior of a FFCC . ASTM C 384 â€“ 90a is readily applicable to air as a medium for sound propagation but its validity for tests under fluidic conditions will have to be ascertained. This paper will describe in detail the impedance tube design considerations, ASTM standard applicability and theoretical framework for tests with fluids as the medium and concerns as applicable to application.

2:15 PM

Break

<u>Other Advanced Material Topics</u>

Room: Sandia Ballroom VII
Session Chair: Tina Nenoff, Sandia National Labs

2:30 PM

Exploring a Battery Worth Its Salt: Ceramic-Salt Interactions in a Low-Temperature Molten Sodium Battery

Erik Spoerke*[1]
1. Sandia National Laboratories

Reliable, safe, and cost-effective batteries are expected to be central elements of the emerging electrical energy grid in the U.S.. We have developed a new class of molten sodium/salt-based batteries, formulated from earth-abundant chemistries, that offers promise for safe and reliable energy storage. Uniquely these molten sodium batteries operate near 100Â°C, a dramatic reduction from the 300Â°C operation of conventional molten sodium batteries, and provide significantly higher voltages (>3.3V) than many other scalable battery chemistries. Comprising a molten sodium metal anode, a NaSICON-based solid-state ion-conducting ceramic separator, and a molten sodium iodide-based metal halide salt catholyte, these innovative batteries introduce a number of unique chemical and materials challenges to scalable implementation. Here, we will specifically discuss recent studies exploring chemical interactions at the interface between the NaSICON ceramic and the molten salt catholyte. We will connect battery cycling performance, selective electrochemical properties, and advanced materials characterization to understand the impact of material composition and catholyte Lewis acidity on key chemical and electrochemical interactions at this critical interface. Understanding these fundamental interactions provides key insights and guidance in the ultimate design of these potentially important batteries.

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2:45 PM

Evacuated photovoltaic thermal (PVT) system for sustainable and efficient cogeneration of heat and electricity

Behnam Roshanzadeh*[1]
1. University of New Mexico

Energy consumption is steadily increasing with the ever-growing population, leading to a rise in global warming. Additionally, the limitation of fossil fuel resources and related environmental issues have been known as pressing challenges for industrialized and developing countries. However, renewable energy installations can provide sustainable solutions if the limitations and challenges of renewables' utilization are addressed properly. One of the drawbacks of photovoltaic systems is the decrease in the PV's efficiency by increasing its surface temperature due to solar irradiation. Photovoltaic thermal (PVT) technology has been introduced to boost the electrical efficiency of the system by cooling the panels. However, in most cases, researchers have investigated unglazed system which has low thermal efficiency. In this paper, the PVT system is encapsulated in an evacuated tube to improve both electrical and thermal efficiencies. The extracted heat can be used for other applications such as domestic hot water supply for buildings or desalination. Most PVT projects focus on increasing electricity production by cooling the photovoltaic (PV). However, in this research, increasing thermal efficiency is investigated through vacuum glass tube encapsulation. The required area for conventional unglazed PVT systems varies between 1.6â€“2 times of solar thermal collectors for similar thermal output. In the case of encapsulation, the required area can decrease by minimizing convective losses from the system. Surprisingly, the electrical efficiency was not decreased by encapsulating the PVT system. The performance of evacuated PVT is compared to glazed and unglazed PVTs, and the result shows a 40% increase in thermal performance with the proposed system. All three systems are simulated in ANSYS 18.1 (Canonsburg, PA, USA) at different mass flow rates and solar irradiance.

3:00 PM

Hydrogen Production by Water/Steam Splitting at Room/Intermediate Temperatures

Meng Zhou*[1], Dr. Hongmei Luo[1]
1. New Mexico State University

Hydrogen is green and sustainable energy, water/steam splitting is one way to produce green hydrogen. Room temperature water splitting is impeded by the sluggish kinetics of Oxygen Evolution Reaction (OER), three strategies have been developed to speed up OER: 1) novel catalyst search; 2) replace OER with other oxidations; 3) temperatures (25 to 65Â°C) related Hydrogen productions. Intermediate temperature (400 - 600Â°C) steam splitting through solid state electrolyser provides a fast path of Hydrogen productions with cheap catalysts. However, delamination and materials degradation significantly reduce the performance and stability of electrolyser, the interface treatment and 3D electrode developments have solved the problems at a certain level while keeping a high Hydrogen production rate.

3:15 PM

Design and Realization of Nanoporous Materials for Acid Gas Separations and Sensing

Matthew Hurlock*[1], Tina M. Nenoff[1]
1. Sandia National Laboratories

The ability to design, tune, and empirically test nanoporous materials allows for the development and commercialization of materials for many different environmental and energy applications. A particular area of interest is the detection, separation, and removal of hazardous gases like CO2, NOx, and SOx. Nanoporous materials such as Metalâ€“organic frameworks (MOFs) and Porous Liquids (PLs) have shown great potential in the separation and sensing of these problematic gases. A fundamental understanding of the structure-property relationships of selective adsorption in these materials is required to better design and improve these technologies. We have shown that MOFs composed of the ligand DOBDC can be tuned to have varying affinities towards acid gases depending on the metal of the structure. We have further used the features of these DOBDC MOFs to develop thin film electrical sensors for the selective detection of acid gases. On the other hand, PLs allow for the use of highly adsorbent materials in flow systems. One PL of interest consists of sorbent ZIF-8 suspended in a solvent mixture. While this PL shows promise as a CO2 adsorption material, the effects of solvent-sorbent interactions on the gas adsorption properties are not well understood. A variety of experimentation have been employed to understand the fundamental structure-property relationships that influence the gas adsorption properties.

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3:30 PM

Mechanochemical synthesis of metal-organic frameworks

Wenyang Gao*[1], Dr. Hongmei Luo[1] Fillipp Edvard Salvador
1. Dept. of Chemistry, New Mexico Tech

Mechanochemical synthesis is emerging as an environmentally friendly yet efficient approach to preparing metal–organic frameworks (MOFs). Herein, we report our systematic investigation on the mechanochemical syntheses of Group 4 element-based MOFs. The developed mechanochemistry allows us to synthesize a family of Hf4O4(OH)4(OOC)12-based MOFs. Integrating [Zr6O4(OH)4(OAc)12]2 and [Hf6O4(OH)4(OAc)12]2 under mechanochemical conditions leads to a unique family of cluster-precise multimetallic MOFs that cannot be accessed by the conventional solvothermal synthesis. Meanwhile, the mechanochemical synthesis also enables us to immediately access metal-catecholate frameworks, a family of redox-active MOFs, based on the linkage of the catechol motif.

3:45 PM

Pressure-less Sintering Approach for Manufacturing NbMoTaWVTix Refractory High Entropy Alloys and First Principles Investigation of the Cohesive Energy and Elastic Properties of Molybdenum

Surya Bijjala*[1], P. Kumar[1], Susan R. Atlas[1]
1. University of New Mexico

Refractory high entropy alloys (RHEAs) potentially provide a compositional space to develop materials for extreme environmental conditions. In particular, NbMoTaWVTix RHEAs have the potential to be used at temperatures where current metallic alloys fail, due to their promising thermal stability and mechanical properties. However, while these RHEAs have the potential to achieve desirable performance targets, engineering challenges in manufacturing may prevent practical structural applications, since current wrought and pressure-induced sintering manufacturing methods are not economically favorable in the context of commercial viability and shape complexity. The pressure-less sintering approach with relatively fewer manufacturing steps has significant economic and scaling advantages for manufacturing RHEAs. We have studied the limit of pressure-less sintering to manufacture dense NbMoTaWVTix. We observed that NbMoTaWVTix with a density as high as 97% can be manufactured with pressure-less sintering utilizing an optimal sintering cycle. The effect of sintering temperature, time, Ti compositions, and the addition of the sintering additive, Ni, on the porosity evolution in the sintered RHEAs will be discussed. We also report on a first principles DFT study to determine the cohesive energy and elastic tensor properties of the RHEA's constituent element molybdenum. The theoretical and computational approach for computing these properties by DFT will be presented.

Advanced and Printed Manufacturing

Room: Sandia Ballroom VIII
Session Chair: Elliot Fowler, Sandia National Labs

1:00 PM

Lattices: Multi-Functional, Reliable (meta)Materials (Invited)

Benjamin White*[1], Brad Boyce[1], Anthony Garland[1]
1. Sandia National Laboratories

Lattices are inseparable from additive manufacturing. From external support structures to novel and fully tunable metamaterials in their own right, lattices give single material printers the ability to print a wide range of effective (meta)material properties allowing for increased part consolidation, faster and cheaper prints, and more efficient higher performing components. Lattices used as standalone materials for their novel properties are also typically reliant on AM as the only feasible production route. This talk will present novel interpenetrating lattices with unique multi-body behaviors that offer advantages as both structural materials, where they can be designed to control damage progression resulting in significant toughening behavior, or as functional materials for load or deformation sensing. Furthermore real lattices contain thousands or even millions of complex features, each with imperfections in shape and material constituency. We show that it is precisely the large quantity of features that serves to homogenize the heterogeneities of the individual features, thereby reducing the variability of the collective structure and achieving effective properties that can be even more consistent than the monolithic base material.

1:30 PM

Characterization of a solid propellant for additive manufacture

Dylan Purcell*[1], Dr. Chelsey Hargather[1]
1. New Mexico Tech, Department of Mechanical Engineering
2. New Mexico Tech, Department of Materials & Metallurgical Engineering

Ammonium perchlorate composite rocket propellant (APCP) is a commonly used solid rocket propellant in commercial and defense applications. Current solid rocket motors are manufactured through a propellant casting process. This method has high associated costs and imposes limitations on the internal structure and composition of the motor, and so an alternative process is desirable. Additive manufacture can address aspects of the process that create the high costs, such as providing on-site manufacture and a reduction of maximum material that needs to be mixed at once, as the process is continuous. In the present work, propellant designed for additive manufacture in an extrusion-driven platform is characterized in terms of viscosity and yield stress of the non-Newtonian uncured material, parameters critical for deposition-based additive manufacture. Spindle and extrusion-based viscometry methods are used to examine the uncured material. Combustion performance is also examined by manufacturing strands of material to study the burn rate. Properties of the final product are compared to tabulated ranges for APCP, and the applications for the material are discussed.

1:45 PM

A New Paradigm in Metal Surface Prep. for High-Throughput Materials Characterization

Elliott Fowler*[1], Shelley Williams[1], Rachel Callaway[1], Matthew Kottwitz[1], Luis Jauregui[1], Michael Melia[1]
1. Sandia National Laboratories

The rapid growth in accessibility of metal additive and advanced manufacturing tools has ignited an exponential rise in demand for characterization to discover process-structure-property (PSP) relationships. Hidden amongst the overflowing demand for characterization is a near universal expectation for performing metallographic preparation of surfaces of interest, from mounting to polishing to etching. Traditional surface preparation is a high-cost, low-throughput bottleneck that ultimately constrains the flow of data generation and reduces the viability of utilizing data science and machine learning in the loop to amplify the discovery of PSP linkages in new materials. In this talk, we introduce a new commercial technology â€“ â€œdryâ€□ electropolishing â€“ which fixtures materials of interest to a spindle (the anode) and spins/shakes them inside a wetted, highly crosslinked, polystyrene sulphonic acid bead media surrounded by a cylindrical titanium net cathode. Furthermore, we discuss several exploitative applications of dry electropolishing to reduce the burden of metallographic surface preparation by orders of magnitude. Finally, we demonstrate how coupling this technique with novel sample and experimental design can shift the paradigm of historically low-throughput microstructural characterization such as melt pool imaging and Electron Backscatter Diffraction (EBSD) from tens to hundreds of measurements per day.

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2:00 PM

Analysis of Pitting Corrosion on Wrought and Additively Manufactured 316L Stainless Steel

Peter Renner[*1], Michael Melia[1], Erin Karasz[1], Kasandra Escarcega Herrera[1]
1. Sandia National Laboratories

Atmospheric corrosion can be difficult to accurately accelerate, and difficulties arise during pit quantification due to the inherent stochastic nature. This research describes the quantification of pitting corrosion on polished samples (800 grit) of wrought and additively manufactured 316L stainless steel when exposed to constant salt (artificial sea water) loading densities and humid environments for times ranging from 1 week to 1 year. The laboratory experiments are compared to an outdoor exposure of similar material on the coast of Florida. After exposure, the corroded surfaces were cleaned of corrosion product and each entire corroded surface was analyzed using white light interferometry to measure pitting damage. The data was post-processed to remove surface variability and â€œfalseâ€□ pits created due to artifacts, allowing for individual pits to be identified and quantified. Finally, the distributions of pits were analyzed and compared across various salt loadings (Âµg/cm2), durations, and relative humidities as a function of wrought and additively manufactured steel through both laboratory experiments and coastal exposure.

Funding statement: SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 SAND #: SAND2022-11407 A

2:15 PM
Break

Session Chair: Kaitlynn Fitzgerald, Sandia National Labs

2:30 PM

Design of Novel Shape Memory and Self-healing Polymer Systems for Additive Manufacturing: Potential Areas of High Impact (Invited)

David Roberson[*1]
1. Polymer Extrusion Lab, The Department of Metallurgical, Materials and Biomedical Engineering, The University of Texas at El Paso

The integration of shape memory polymers with additive manufacturing (AM) platforms has led to what many refer to as â€œ4D Printing.â€□ Well-planned materials selection in the design of novel material systems not only furthers this growing branch of digital manufacturing, but opens the door to a broad range of applications that can potentially impact a wide variety of fields. The work presented here covers recent research efforts in the development of novel shape memory polymer systems for the AM platform of fused filament fabrication (FFF). Materials selection criteria will be discussed as well as the determination of critical temperatures related to shape memory mechanisms. Design strategies for application specific shape memory polymers will also be covered where impact in the areas of biomaterials and environmental sustainability will be demonstrated. Materials characterization efforts will also be presented including phase characterization via scanning transmission electron microscopy (STEM). Finally, the relationship between shape-memory and self-healing properties of polymers will be explained along with the development of a novel material property.

3:00 PM

Rapid 3D printing of Nd:YAG ceramic for lasing media

Luyang Liu[*1], Xiangfan Chen[1]
1. School of Manufacturing Systems and Networks, Arizona State University

Polycrystalline transparent yttrium aluminum garnet (YAG, Y3Al5O12) ceramic doped with rare-earth metals such as neodymium (Nd: YAG) has broad applications as a lasing medium. In this study, we developed a new fabrication method for Nd: YAG-based lasing media by solvent-gelation reaction, micro-continuous liquid interface printing (Î¼CLIP) with post heat treatment processes. With the resolution of 5.8 Î¼mÂ·pixelâ€“1 and the printing speed of 10 Î¼mÂ·sâ€“1, the Î¼CLIP system can fabricate multi-scaled Nd: YAG green bodies efficiently. Characterization results show that after the post heat treatment processes the fabricated samples photoluminesce at 1064 nm pumped by 532 nm laser. This new approach is beneficial for developing lasing media with customized, sophisticated 3D structures within a shorter timescale.

3:15 PM

Heat treatment effects on mechanical properties of Wire Arc Additive Manufactured Ti-6Al-4V

Natalia Saiz*[1], Jonathan W. Pegues[1], Shaun R. Whetten[1], Andrew B. Kustas[1], Tyler Chilson[1]
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Directed energy deposition (DED) is an attractive additive manufacturing (AM) process for large structural components. The rapid solidification and layer-by-layer process associated with DED results in non-ideal microstructures, such as large grains with strong crystallographic textures, resulting in severe anisotropy and low ductility. Despite these challenges, DED has been identified as a potential solution for the manufacturing of near net shape Ti-6Al-4V preforms. In this work, we explore several heat treatment processes, including HIP, and their effects on tensile properties of wire arc additively manufactured (WAAM) Ti-6Al-4V. A high throughput tensile testing procedure was utilized to generate statistically relevant data sets related to each specific heat treatment and sample orientation. Results are discussed in the context of microstructural evolution and the resulting fracture behavior for each condition as compared to conventionally processed Ti-6Al-4V.

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Keywords: Additive manufacturing, laser engineered net shaping, process-structure-property relationships, Ti-6Al-4V

3:30 PM

Building Microwave Dielectric Ceramics and Metallization via Dry Aerosol Deposition

Alex Valdez*[1], Paul Fuierer[1]
1. New Mexico Institute of Mining and Technology

Dielectric ceramics with tunable relative permittivity (K) and high quality factor (Q) is critical for modern microwave and millimeter wave communication technologies. Hybrid and additive manufacturing (AM) techniques are required to build filters, passives, antennas, resonators, and custom circuits. Dry aerosol deposition (DAD) is a novel kinetic AM process that can produce thick films and low-profile 3D dielectric ceramic structures on practical substrates at room temperature. Our recent work concerns $BaNd_2Ti_4O_{12}$ (BNT), a complex perovskite microwave dielectric with a high-K, high-Q, and low thermal coefficient of resonant frequency. Microstructural analysis and dielectric properties of DAD BNT thick films are compared with bulk sintered BNT. SEM and AFM show that the thick films are fully dense and have excellent adhesion. It is also shown that the same DAD machine can deposit copper on dielectric ceramics to build high-frequency ring resonators and typical metallization.

3:45 PM

Process-Structure-Property Evaluation of Laser-Hot Wire CP-Ti Grade 2

Hannah Sims*[1], John J Lewandowski[1]
1. Sandia National Laboratories
2. Case Western Reserve University

The effects of different processing conditions on the chemistry, microstructure and mechanical properties of CP-Ti Grade 2 processed via a wire-based additively manufactured laser hot-wire (LHW) process were determined. Biomedical grade CP-Ti Grade 2 wire was used for wall deposits conducted at both Lincoln-Electric Company and ORNL/MDF. Initial builds exhibited process-induced defects from insufficient pass overlap and oxygen contamination that affected both the location and orientation dependence of mechanical properties. Single bead deposits conducted over a range of process conditions (power, velocity, travel speed) were used to refine the LHW deposition parameters that were subsequently used to produce more homogenous and nominally defect-free material. Tension, hardness, Charpy impact toughness, fatigue crack growth, and J-integral fracture toughness were determined by excising samples from all builds at different locations and different orientations. Fracture surfaces were analyzed by SEM while microstructures were analyzed with both optical and EBSD techniques. Both differential scanning calorimetry (DSC) and LECO oxygen analysis were used to document the beta transus in different builds and correlate that with the resulting oxygen content.

The initial builds exhibited process-induced defects due to insufficient pass overlap in addition to oxygen contamination that exceed the Grade 2 specification. While these defects and differences in oxygen concentration produced variations in mechanical properties that were also dependent upon the sample location and orientation, fracture surfaces were ductile, and properties were in the range of conventionally processed material despite being tested in the as-deposited condition. The microstructure features were thin laths of alpha near the bottom of the build that coarsened into large alpha grains higher in the build. The optimized builds produced at ORNL/MDF used guidelines developed from the single bead deposits, met oxygen specifications for CP-Ti Grade 2, and were nominally defect-free. The mechanical properties were again both location and orientation-dependent but controlled by differences in microstructural features and sizes. The thin alpha laths near the bottom of the builds produced the best mechanical properties. The mechanical properties of all builds compared favorably to more traditionally processed (e.g., cast, wrought, welded) material as well as other CP-Ti Grade 2 that had been additively manufactured.

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Poster Session
Room: Main Lobby

4:00 PM

Undergraduate Student

U1 - Development of a pyrotechnic initiator ink for additive manufacturing methodology

Benito Silva*[1], Dr. Chelsey Hargather[1]
1. New Mexico Tech Department of Materials and Metallurgical Engineering

The purpose of this study is to develop a pyrotechnic initiator ink formulation and to develop an accurate deposition process for the ink. The main focus of the ink formulation is to demonstrate multi-point initiation of an energetic substrate. Additionally, controlling the burning profile of the energetic substrate is desired. Thermites have a high thermal output with low gas emission, and are the ideal energetic for the ink formulation. Three thermitic formulations are developed using aluminum as a fuel and either barium nitrate, strontium nitrate, or manganese (IV) oxide as oxidizers. The oxidizer and fuel mixture is combined with a stoichiometric mixture of iron and sulfur in order to help stabilize and control the burning of the thermite. The material is bound in a polymeric binder. These three formulations are mixed and put into molds, cured, and tested based on the combustion rate and thermal output. The barium nitrate formulation has the highest thermal output of about 1250 °C and the highest burn rate of about 0.079 in/sec. The manganese (IV) oxide formulation had the most uncontrolled burn profile and lowest thermal output, making the formulation not viable for further testing. The strontium nitrate sample has a relatively controlled burned profile with a high thermal output.

U2 - Additive Manufacturing (AM) Of Thermoset Polymers

Nicolas Monk*[1], Samuel Leguizamon[1], Leah Appelhans[1]
1. Sandia National Laboratories

3D printing with thermoset materials is valuable because of the ability to form chemical bonds between layers, enhancing interlayer adhesion and homogeneity. Thermoset materials are also known for their good thermal and mechanical properties. We demonstrate two formulations for the AM of thermoset materials. The first system uses dicyclopentadiene (DCPD), which is polymerized through ring opening metathesis polymerization (ROMP) and has a high toughness. However, with existing photoinitiated catalysts the rate of polymerization was too slow for AM. We found that with the addition of a photosensitizer we could achieve a high rate of ROMP of DCPD, which allows us to print via Direct-Ink-Write and vat polymerization printing. Our second system is a dual-cure epoxy/acrylate resin, which uses both light and thermal activation for polymerization. In this presentation we will cover the different components of each system and how changing the constituents and stoichiometries can change the print performance. Analyzing the kinetics of our systems using photorheology we can determine our optimum printing formulation. We also use photorheology to determine how UV light intensities affect the properties of the polymer network. Using the photorheology results we can rapidly screen formulations for printability which allows us to use less material and time to identify promising resin candidates.

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U3 - Evacuated photovoltaic thermal (PVT) system for sustainable and efficient cogeneration of heat and electricity

Behnam Roshanzadeh*[1], Gowtham Mohan[1]
1. University of New Mexico

Energy consumption is steadily increasing with the ever-growing population, leading to a rise in global warming. Additionally, the limitation of fossil fuel resources and related environmental issues have been known as pressing challenges for industrialized and developing countries. However, renewable energy installations can provide sustainable solutions if the limitations and challenges of renewable utilization are adequately addressed. One of the drawbacks of photovoltaic systems is the decrease in the PV's efficiency by increasing its surface temperature due to solar irradiation. Photovoltaic thermal (PVT) technology has been introduced to boost the electrical efficiency of the system by cooling the panels. However, in most cases, researchers have investigated unglazed system which has low thermal efficiency. In this paper, the PVT system is encapsulated in an evacuated tube to improve both electrical and thermal efficiencies. The extracted heat can be used for other applications such as domestic hot water supply for buildings or desalination. Most PVT projects focus on increasing electricity production by cooling the photovoltaic (PV). However, in this research, increasing thermal efficiency is investigated through vacuum glass tube encapsulation. The required area for conventional unglazed PVT systems varies between 1.6–2 times of solar thermal collectors for similar thermal output. In the case of encapsulation, the required area can decrease by minimizing convective losses from the system. Surprisingly, the electrical efficiency was not decreased by encapsulating the PVT system. The performance of evacuated PVT is compared to glazed and unglazed PVTs, and the result shows a 40% increase in thermal performance with the proposed system. All three systems are simulated in ANSYS 18.1 (Canonsburg, PA, USA) at different mass flow rates and solar irradiance.

U4 - Viscosity Characterization and Modeling of Thermite Energetic for 3D Printing

Hannah Morgan-Smith Myers*[1], Chelsey Hargather[1]
1. New Mexico Tech Department of Materials and Metallurgical Engineering

Additive manufacturing is a useful tool that has yet to be thoroughly applied to the manufacturing of energetic materials. Conventional manufacturing of energetics requires specialized molds and equipment, which are costly and make prototyping difficult. 3D printing does not require molds, which dramatically reduces cost and allows specialized shapes to be more easily manufactured. Additionally, rapid prototypes can be produced using 3D printing, which is beneficial. In order to engineer a 3D printable material, a material with high viscosity and yield stress is required, which allows the material to hold a rigid shape once printed. This project focuses on characterizing the viscosity of an energetic system using a rotational viscometer. The end product of this project will be a fully 3D printable energetic material with easily customizable parameters based on the requirements of the system. Changes to the particle size ratios, binder system, and catalyst concentration will be done to optimize printability for given applications. In the present work, experimental viscometry procedures have been established for curing and non-curing energetic systems. For non-newtonian fluids of high viscosity, it is critical that proper mixing and recovery are conducted before any rheological data can be gathered.

U5 - Soldered Tensile Failure Stress of Ceramics in Multilayered Ceramic Capacitors

Titus Jamar Rogers*[1], Kevin T. Strong Jr[1], Scott Grutzik[1], Jeier Yang[1], Rebecca Wheeling[1],
1. Sandia National Laboratories

Ceramics are known to fail in a stochastic manner due manufacturing flaws (pores, inclusions, machining defects, etc.). The “weakest link” analogy is used to describe failure as occurring from the largest flaw in the area of highest stress. Because of this effect a single value tensile strength cannot be used for predicting strength of ceramic parts. Weibull strength size-scaling can be successfully used to predict the strength of a ceramic part subjected to tensile stress from a standard laboratory flexure test. However, it is unknown whether this can be applied when the ceramic has a complex thermal residual stress field from a joining process such as soldering. The ceramic dielectric from multilayered ceramic capacitors (MLCCs) was chosen as it is a very common commercial ceramic that is soldered. Tape cast coupons were acquired from the manufacturer and equibiaxial flexure was used to measure the tensile strength. Additional samples were fabricated with a soldered copper disc in the center of the coupon. The area with the soldered disc was place on the tensile side of the equibiaxial flexure fixture to measure the solder strength. Finite element analysis (FEA) was used to simulate the solder stress of the ceramic coupons. The simulated ceramic was then placed in equibiaxial stress the same as the experimental fixture. A probability of failure was predicted using the Weibull parameters from the unsoldered ceramic strength tests. The experimental and computation results are compared.

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U6 - Rapid Detection of Viruses via Metal Organic Frameworks (MOFs)

Elizabeth Zapien*[1], Elizabeth A. Nail[1], Andreana M. Nourie[1], Kauryn A. Datcher[1], Leah N. Appelhans[1], Kimberly S. Butler[1]
1. Sandia National Laboratories

Rapid, accurate detection of pathogens is critical for public health and safety. Many current methods of detection have shortcomings. Some require the use of expensive and complex instruments or must be stored in a controlled temperature environment. In this study, we tested a new detection method to try to solve some of the problems with existing methods of viral detection. With the use of metal-organic frameworks (MOFs) as a biosensor, we tested to see if rapid, accurate viral detection was possible.

The MOF biosensor system consists of the MOF which will quench the probe fluorescence, and the DNA probe which is sequence specific to the virus we want to detect. When the system is exposed to the virus, the probe will be released from the MOF which causes the fluorescence to be recovered.

We tested crystalline and amorphous Cu dithiooxamide MOFs using an HIV-virus specific sequence. Both samples were able to quench the probe fluorescence at the same concentration. We next introduced the target sequence and fluorescence was recovered in both samples, showing that the MOF/probe system could be successfully used for detecting HIV-specific DNA sequences. Next, probes designed to target SARS-CoV-2 were tested. The fluorescence was quenched with both MOFs. Our next step will be to add the target sequence and see if the fluorescence can be recovered.

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U7 - Electron Backscatter Diffraction Analysis of Additively Manufactured Steel Grains

Landon Schnebly*[1]
1. Brigham Young University

Additive manufacturing is an emerging technology that allows 3D-printing of steel structures by melting a steel powder with a high-powered laser. The resulting melt pool affects both the grain size and amount of columnar growth. Electron Backscatter Diffraction analysis across three samples manufactured with the same parameters shows that the microstructure of an additively manufactured steel part can be accurately predicted when the fabrication parameters are kept constant.

U8 - Impact of Relative Humidity and Salt Loading Densities on the Localized Corrosion Behavior of Additively Manufactured and Wrought Stainless Steels

Kasandra Escarcega Herrera*[1]
1. Sandia National Laboratories

Laser beam powder bed fusion (LB-PBF) is a modern manufacturing technique for metal components. Stainless steels, like 316, are commonly used in LB-PBF machines. Wrought stainless steels have been developed to exhibit good general corrosion resistance. However, in chloride rich environments such as marine environments, they are susceptible to localized corrosion and pitting. The microstructure created by the non-equilibrium LB-PBF process is vastly different than it's wrought counterpart, and this can cause differences in their respective corrosion behavior. This study will investigate the localized corrosion susceptibility of wrought and LB-PBF 316L stainless steel exposed to different relative humidities, 40 and 76%, with fixed contaminant levels of artificial seawater, 20 and 300 µg/cm2. Analysis of post exposure corrosion damage will be quantified with electron microscopy and optical profilometry. A new protocol will be introduced to analyze pit depth and volume from the surface topology measurements using the MountainMaps software suite.

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U9 - Assessing Cellular Internalization Pathways for Lipid Coated Silica Nanoparticle Mediated Nucleic Acid Delivery Platforms

Johanna Tsala Ebode*[1]
1. Chemical and Biological Engineering

The use of various nanoparticles for the delivery of nucleic acids in gene therapy is a promising approach for the treatment of diseases resulting from genetic mutations. While promising, this technology has many biological barriers for the effective delivery of nucleic acids. More specifically, internalization and intracellular pathways in a cell dictate the ultimate fate of the nanoparticle and nucleic acids which impacts the overall effectiveness of the therapeutic approach. Endocytosis is a path by which cells take in substances from outside and submerge them in a vesicle. Upon internalization on the plasma membrane, lipid-coated silica nanoparticles serving as nucleic acid carriers are intended to use this pathway to reach the cytosol and release the nucleic acid in the nucleus to target a specific gene of a disease. Silica is considered safe by the FDA and engineered lipid coatings are expected to improve the biocompatibility of the particles. Bare lipid-coated silica nanoparticles, however, often get trapped and then degraded by the enzymes contained in the endosomes/lysosomes, thus preventing the desired RNA from reaching its intended destination, meaning a modulation of the particles is needed to enable an endosomal escape. In our study, we investigated the internalization pathway of lipid-coated silica nanoparticles in LNCaP cells, a prostate cancer cell line. Our approach involves modulating lipid-coated silica nanoparticles to improve their characteristics using two different systems and look at the colocalization of those particles versus bare lipid-coated silica nanoparticles with endosomal markers using confocal microscopy to assess whether an endosomal marker occurs and how our lipid-coated silica nanoparticles are internalized.

U10 - Mesoporous Organosilica Nanoparticles as a promising carrier to enhance efficacy/safety ratio for advanced ovarian cancer

Marian Olewine*[1], Paulina Naydenkov[1], Rita Serda[1], Jeffrey Brinker[1], Achraf Noureddine[1]
1. Chemical and Biological Engineering

According to the American Cancer Society many anti-cancer drugs including chemotherapeutics (such as paclitaxel, irinotecan, and thioguanine) and targeted therapeutics (Afatinib and Olaparib) used in clinics are hydrophobic and suffer from low bioavailability so higher repetitive doses are needed. For these reasons, biocompatible carriers are needed to protect the drug and increase its bioavailability. Advanced stage ovarian cancer in women involves intraperitoneal injection (IP) of high doses of chemotherapeutic drugs which generally results in severe side effects. Therefore, new drug combination that lessen the chemotherapy dose but maintain same efficacy are attractive. Afatinib, a tyrosine kinase inhibitor is currently used as a first line treatment for non-small cell lung cancer (NSCLC) and being investigated for Her2 positive breast cancer. Serous epithelial ovarian cancer express Her2/neu mutations [1], indicating that Afatinib can be a promising therapy. We have developed lipid-coated organosilica nanoparticles that efficiently load the hydrophobic drugs and screened the efficacy to BR5 mice ovarian cancer cells of various drug combination in presence of afatinib. We have used transmission electron microscopy and ZetaSizer to assess the shape and colloidal stability of the nanoparticles, cell titer glo assay for in vitro efficacy of the drug combination, plate reader and nanodrop of drug loading, IVIS for in vivo studies where preliminary data has shown promising results in afatinib and paclitaxel combination loaded in nanoparticles on IP injected mice.

[1] Alvarez et al Gynecol Oncol Rep. 2019 Aug; 29: 70–72

U11 - Development of long wavelength quantum dots for single photon applications.

Carter Heinrich*[1]
1. University of New Mexico

InAs Stranski-Krastanov (SK) quantum dots have been used for single photon emitters. The SK growth mode involves the growth of a planar wetting layer of InAs on a substrate like GaAs, and subsequently the high mismatch drives the growth three dimensional leading to an ensemble of nanoscale islands or quantum dots. This growth phenomenon has been observed in a few material systems; however, InAs on GaAs has been the most widely used embodiment of this growth resulting in lasers, solar cells and detectors.

The coverage of InAs that is used for quantum dots ranges from 1 ML which is a pure wetting layer to up to 2.7 MLs. Beyond this, the dots experience Oswald ripening and result in photonically inactive quantum dots. This translates to a wavelength range of ~ 1000 nm to 1250 nm.

While these quantum dots are typically very high in density at > 10^10 dots/cm^2, through growth methods the density can be reduced, and using advanced microscopic techniques a region with a few quantum dots can be probed.

In this paper we attempt to increase the emission wavelength of InAs quantum dots to telecommunication wavelengths of 1.33 µm and subsequently to 1.55 µm. To do this, we must be able to grow larger quantum dots and that will require reduced mismatch between the quantum dot and the underlying substrate. We therefore employ a metamorphic buffer on GaAs comprised of step graded AlGaAsSb. The results presented will include XRD and TEM based characterization of the buffer along with AFM and photoluminescence-based analysis of the quantum dots.

U12 - Applications of Coatings for the Mitigation and Repair of Stress Corrosion Cracking on Spent Nuclear Fuel Canisters

Makeila Maguire*[1], Andrew Knight[1], Brendan Nation[1], Rebecca Schaller[1], Charles Bryan[1]
1. Sandia National Laboratories, Albuquerque, NM 87123 USA

There are currently 81 Independent Spent Fuel Storage Installations located across the United States, many of which are in coastal regions near marine environments. As spent nuclear fuel (SNF) cools due to radioactive decay over time, the relative humidity on the canister surface can increase. Under these conditions, deliquescence can occur as a consequence of salt deposition on the canister surface, leading to the formation of stable, corrosive, Cl^- rich brines on stainless steel (SS) dry storage canisters (DSC). The presence of a brine can lead to localized corrosion of the SS canister, which with increased storage times, could increase the probability for stress corrosion cracking (SCC) to occur, where the greatest possibility exists along canister welds. While recent research has greatly improved our understanding of the fundamental mechanisms that could result in SCC, this work focuses on possible prevention, mitigation, and repair techniques to help protect the SNF DSCs against potential SCC. To do so, the properties of 11 coatings (5 polymeric, 5 organic/inorganic hybrid ceramic, 1 Zn-rich primer) from 4 different coating manufacturers were evaluated by performing adhesion and scratch tests on coated, 3”X6” 304L austenitic SS coupons, to determine their mechanical robustness. Mechanical robustness is a property that has been considered to be important for a mitigation and repair strategy, especially if the canister will need to be moved once a coating has been applied. In general, polymer coatings such as polyetherketoneketone or polyurea-polyimide-phenolic resin composites produced favorable results with high pull-off forces and epoxy level failure during adhesion testing, as well as sustained adhesion following scratch testing. In contrast, the ceramic and Zn-rich primer coatings experienced multiple failure types in addition to low adhesion strength and scratch resistance—which were negatively impacted by atmospheric exposures. By determining the mechanical limits of these coatings, an informed approach to coating SNF DSC can be implemented to lengthen their lifetime and decrease canister susceptibility to SCC.

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U13 - Improving Anti-Icing Coatings Though the Exploration of Ionomer Film Blends

Annika Jansen*[1]
1. Advanced Materials Laboratory

Ice buildup and accumulation on machinery and infrastructure such as powerlines and solar panels can make operation difficult and hazardous. Common methods for removing accumulated ice are energy-intensive and require active maintenance; a preferred solution would be to engineer a surface that inhibits ice formation and/or lowers the adhesion force of ice such that it can be passively removed. There has been a great deal of work in the literature developing such “icephobic” coatings, however these typically lack the durability required for long-term deployment. In this study, we explored a new system of icephobic coatings based on ionomer films blended with low molecular weight glycols and divalent cationic salts. It is expected that the cationic salts will act as dynamic crosslinkers in the ionomer film leading to the ability of coatings to self-heal damage and grant higher durability.

U14 - Inhibiting Effect of Nitrate on Chloride Induced Corrosion of Stainless Steel 304

Jason Snow*[1], Ryan Katona[1], Makeila Maguire[1], Charles Bryan[1], Andrew Knight[1], Rebecca Schaller[1]
1. Sandia National Labs

Chlorides and nitrates can be present in significant quantities in the atmosphere, with high nitrate concentrations common in settings such as rural farming areas due to the widespread use of nitrate-containing fertilizers. These anions deposit on exposed surfaces and wet when the ambient relative humidity is greater than the salts’ deliquescence points. Chlorides are known to typically accelerate localized corrosion of austenitic stainless steel while nitrates, at certain concentrations, have been found to inhibit corrosion. Therefore, it is important to determine what influence the nitrate to chloride ratio has on pitting intensity and morphology under various exposure conditions. To gain a general understanding of this relationship, full immersion cyclic potentiodynamic polarizations have been conducted at various temperatures, scan rates, and salt ratios on 304 stainless steel. Additionally, 304 coupons with deposited droplets of various sizes and concentrations were exposed to a variable RH environment, and the resulting pits were examined with an optical microscope and SEM.

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Graduate Student

G1 - Characterization of Polyacrylamide Hydrogel Formulations as an Optimal Biomimetic Material for Traumatic Brain Injuries

Anthony Baker*[1], James Angelos[1], Eric Galindo[1], Sorcha Sterritt[1], Michaelann Tartis[1]
1. New Mexico Institute of Mining and Technology

To study damage mechanisms and cellular responses in traumatic brain injuries, biomaterials are needed to match the bulk and cellular microenvironment. Hydrogels that resemble the rheological properties of in vivo tissue allow for observation of biofidelic cell responses after a blunt impact in ex vivo settings. Polyacrylamide hydrogels are ideal because they are bioinert and have tunable rheological properties, specifically the storage modulus, loss modulus, and tan delta. Monomer to crosslinker content and linear acrylamide chains were manipulated to create hydrogels to mimic the gray and white matter of brain tissue. In this study, hydrogels were analyzed with a stress-controlled oscillatory rheometer and compared with ex vivo tissue values from literature. Full scale brain phantoms were scanned using Magnetic Resonance Elastography and compared with in vivo data from healthy human volunteers. Hydrogel formulations resulted in a storage modulus between 1 and 4 kPa and a loss modulus between 0.2 and 1 kPa, while maintaining tan delta values between 0.15 and 0.25. Atomic Force Microscopy was utilized to assess microrheological properties of hydrogels and compare them to values from an oscillatory rheometer. Fibroblasts will be seeded on these hydrogels to mimic white and gray matter tissue. Future directions are to assess the neurophysiological response of cells seeded on hydrogels with different rheological properties during a traumatic brain injury deformation scenario.

G2 - High frame rate acoustic and optical imaging of a polyacrylamide human head model under blunt impact for cavitation detection

Eric Galindo*[1]
1. New Mexico Tech

Despite decades of research, damage mechanisms associated with blast and blunt traumatic brain injuries are not well understood. To better understand the damaging mechanisms of TBIs, one being cavitation, a head model with agreeable deformation properties compared to in-vivo brain tissue is needed. Currently, many models presented in the literature do not incorporate anatomical features of the human brain. In this study, the fabricated phantom includes the gray and white matter brain layers while adding simplistic geometrical structures, such as the gyri, sulci, and ventricles. The polymeric hydrogel phantom is composed of polyacrylamide (PAA), known for its crosslinked network and tunable mechanical properties. Therefore, a 7 (w/v) % and 10 (w/v) % 60:1 monomer to crosslinker formulation portrays the gray and white matter, respectively, while providing optical transparency. The phantom's stiffness was characterized through classical oscillatory parallel plate rheology at low frequencies and magnetic resonance elastography (MRE) at higher frequencies compared to a healthy human volunteer. The PAA phantom is enclosed in a 3-D printed skull with cerebrospinal fluid (CSF) similar to the mechanical properties of human cranial bone. The head model underwent a series of blunt impacts where high-speed optical and acoustic imaging detected the resulting formation, location, and persistence of cavitation bubbles caused by pressure differentials.

G3 - Fiber Optic Tethered Micro-Tools Built from Stiff/Soft Composites

Georgia Kaufman*[1], Jorge Jimenez[1], Michael Gallegos[1], Emily Huntley[1], Holly Golecki[1], Bryan Kaehr[1]
1. Advanced Materials Laboraotry, Sandia National Laboratories

Soft robots built from compliant materials enable manipulation of delicate objects by mimicking the musculoskeletal architectures of biological systems. Though many concepts of soft robotics have been successfully demonstrated at organism scale, scaling materials, fabrication approaches and ultimately functions down to the microscale remains a challenge. In this work, we investigate additive manufacturing of microgrippers based on bioinspired designs coupled with environmentally actuated hydrogels to form hybrid microsurgical tools. We aim to develop robust micro-grippers integrated into imaging/optogenetic devices at the scale of single fiber optics and individual biological cells to enable single cell manipulation or localized delivery. Using multiphoton lithography, we fabricate resin grippers and scissors that incorporate inert skeletal components. Hydrogels that respond to changes in temperature, pH and light are used to control device movements, and are fabricated in situ from the light output of the tip of the fiber. We evaluate the response time and cyclability of grippers. By leveraging gripper geometry, surface treatments, and hydrogel chemistry, we iterate on designs to optimize for specific functions. Finally, we designed microgrippers that enable photothermal transduction within a thermally responsive gel actuator fabricated on the tip of a 200-micron diameter core fiber and demonstrate capture and release of microscale objects. Overall, this work provides a foundation to integrate stimuli responsive mechanical functions with micro-scale optical devices.

G4 - Formation and Interrogation of a Modeling Excel Database for Sorbent Preconcentration

Lisa Caravello*[1], Joshua Whiting[1], Philip Miller[1], Jason Sammon[1], Bryan Weaver[1]
1. Sandia National Laboratories

Volatile organic compounds (VOCs) are of great interest and the subject of much research, as they can be used in various applications, including indicating hazardous environmental conditions, as biomarkers for disease, and for military uses such as detection of chemical warfare. Preconcentrating this class of analytes is necessary as they can be elusive with simple sampling techniques. VOCs are often captured using sorbents in thermal desorption tubes as preconcentrates prior to analysis, commonly gas chromatography mass spectroscopy (GCMS). While this approach is common there is a gap in knowledge in behavior of materials used as sorbents i.e., if they will retain an analyte of interest appropriately. There is limited literature on single sorbent beds, and many researchers rely on method development using trial and error. While this approach is reliable, it is often time consuming and requires resources that could be used elsewhere in the research. A general tool that can be applied to any analyte would improve understanding of single bed sorbents and would be beneficial to the scientific community.

In this research I seek to eliminate speculation and unknown variables for analyte and sorbent combinations by creating a predictive database. This database models how analytes will elute through specific preconcentrator sorbents, using retention index. The predictions from this database are then interrogated with laboratory experimentation.

G5 - Fatigue Life of Welded 304L Stainless Steel

Trent Whiteside*[1], Dr. Tariq Khraishi[1], Dr. Pankaj Kumar[1]
1. UNM ME Graduate Student

A collection of welded 304L stainless steel coupons consisting of 3 weld types was cyclically tested uniaxially in load control to determine the expected fatigue life, to characterize the resulting microstructure, and to ascertain the most prevalent cause of eventual failure. All tests were conducted entirely in tension using a Mechanical Testing System (MTS) test frame at a frequency of 5 Hz and stress ratio $R = 0.1$. To understand the failure process, SEM analysis is ongoing to characterize the microstructure in three regions including the fusion zone (FZ), heat effected zone (HAZ), and parent material (PM). Cyclic fatigue data was analyzed to determine if the observed stress vs cycle (or SN) behavior is in close agreement with a known fatigue life model. A comparison of the fatigue life of welded and unwelded specimens strongly suggests that welding 304L decreases its fatigue life considerably.

G6 - Fundamental Studies and Functional Applications of Mechanotropic Phase Transitions

Jeremy Herman*[1], Timothy J. White[1]
1. Department of Chemical and Biological Engineering, University of Colorado Boulder

Mechanotropic phase transitions have been observed in amorphous polymer networks prepared with large concentrations of liquid crystalline units. Mechanical force transitions the materials from the amorphous state into an aligned nematic phase. These materials show promise as dynamic optical films and for their elastocaloric effects. This work details fundamental studies of these mechanotropic phase transitions as well as further experiments to enhance optical and elastocaloric functionality.

G7 - Synthetic Biology Enabled Modification of Bone Cells and the Impact on Bone Mineral Formation.

Dulce C. Hayes*[1], Kimberly Butler[1], Kalista Blake Pattison[1], Jerilyn A. Timlin[1]
1. Sandia National Laboratories

Bone is a hybrid inorganic-organic material composed primarily of the mineral hydroxyapatite and the protein collagen. The ability of bone to remodel and regenerate makes it attractive for advanced material applications. Bone tissue is composed of three types of cells; osteoblasts (form bone), osteocytes (sense mechanical stress) and osteoclasts (remove bone). In vivo, bone continuously remodels in response to RANKL/RANK/OPG signaling between osteoclasts and osteoblasts. Abnormal signaling in bone results in bone metabolic diseases caused by the imbalance between bone formation and bone resorption. For example, osteosarcoma can produce osteolytic lesions, resulting in excessive destruction of bone. In this study we engineered osteoblasts to alter the levels of signaling molecules in the RANKL/RANK/OPG pathway and assessed the effect on osteoclast induction and resorption. K7M2, osteoblast cells were genetically modified to overexpress osteoprotegerin (OPG) using lentivirus transduction. OPG overexpression was confirmed at the gene and protein level with Polymerase Chain Reaction (PCR) and Enzyme-Linked Immunoassay (ELISA) assays respectively. RAW 264.7, monocyte cells were induced with K7M2-OPG conditioned medium with RANKL and confocal fluorescence microscopy was used to confirm the formation of osteoclasts. Osteoclast functionality was confirmed with a resorption pit assay using calcium phosphate as synthetic biomimetic material. Preliminary results show that engineering OPG is sufficient to alter the osteoclastogenic capacity of K7M2 cells. This work represents an important initial step in utilizing synthetic biology to elucidate the mechanisms that inhibit osteoclastogenesis in osteosarcoma in-vitro.

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G8 - Development and characterization of recyclable epoxy/refractory plasmonic nanoparticles for additive manufacturing

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Thermoset epoxy polymers are non-recyclable due to their irreversible crosslinked structure. We develop thermally reversible epoxies by incorporating dynamic covalent bonds like diene-dienophile linkages initiating Diels' Alder reaction chemistry. However, the lack of localized heating precision and low thermal conductivity of epoxies can make the recycling using bulk heating process ineffective. We apply refractory plasmonic inexpensive Titanium Nitride (TiN) for converting the incident light to localized heat leading to depolymerization of epoxies at targeted areas. Titanium nitride nanoparticles show strong plasmonic properties due to their metallic behavior and is attractive due to their superior thermal stability and broader solar light absorption features. The incorporation of titanium nitride nanoparticles in the reversible epoxies provide several advantages: (1) application of solar light to liquefy(depolymerize) the epoxy for reprocessing, (2) targeted repair of defects on a 3-D printed epoxy structure, (3) fast curing of epoxy using light, required for their 3-D printing applications, and finally (4) smoothening the rough surface of the final products. We are functionalizing TiN nanoparticles with thiol group via sonochemical method, for better dispersion of TiN nanoparticles in the epoxy matrix. The functionalization of nanoparticles is confirmed using FTIR spectroscopy. We also characterized the nanoparticles dispersion in the composites and the surface roughness of the composite structures using Atomic Force Microscopy. The surface roughness of the structure could be reduced by 45% by melting the top surface of the structure using solar irradiation.

G9 - Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy

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Thermoset polymers such as epoxy resins have been used extensively in coatings, structural, electronics, and adhesive applications. Unlike thermoplastic polymers, the end-of-life products of these polymers cannot be repaired or recycled by applying heat as this will cause the material to be damaged rather than melt. We synthesized a reversible epoxy containing Diels-Alder adducts that is capable of depolymerizing at higher temperatures and repolymerizing at lower temperatures, allowing the epoxy to become recyclable. Additionally, photothermal plasmonic titanium nitride nanoparticles (TiN) are incorporated to the epoxy matrix. When irradiated with solar light, the nanoparticles will induce heating at the nanoscale that is rapidly delivered to the Diels-Alder adducts, causing quick depolymerization in a specific area if desired. These epoxy composites were irradiated with different levels of light intensity from a solar simulator; light intensity was varied from 142 mW/cm2 to over 1000 mW/cm2. Reversible epoxies/nanoparticle composites containing different wt.% of TiN nanoparticles (0, 0.2, 0.5, and 0.7 wt.%) were tested for their light absorbance as well as photothermal efficiency. Optical microscopy is used to study the in situ melting of the epoxy composites under solar simulator. Both the nanoparticle loading as well as the light intensity were optimized to determine the optimal conditions for melting, which is important for the reprocessing and recycling of the epoxy. Results indicate that solar light concentrated with a lens can produce sufficient intensity to melt TiN nanoparticle-laden epoxy. This procedure could be increased from the laboratory scale and used to extend the lifetime or recycle products.

G10 - Enhancing immunogenicity by displaying a Universal T cell Epitope On the Surface of A Virus Like Particle

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1. Bryce Chackerian

Virus-like particles (VLPs) consist of viral structural proteins that, when overexpressed, spontaneously self-assemble into particles that are antigenically indistinguishable from infectious virus or sub viral particles. VLPs can be considered as dense, repetitive arrays of one or more protein subunits with properties that are highly advantageous for use as stand-alone vaccines or as vaccine platforms. Using VLPs to display PADRE a universal T cell epitope can enhance

immunogenicity of the vaccine while also providing lasting protection against the pathogen of interest.

G11 - Rational Design of Silica-Based Nanoparticles for Overcoming Barriers of siRNA Delivery in Prostate Cancer Applications

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The use of exogenous siRNA technology to modulate aberrant protein expression resulting from genetic mutations is a promising therapeutic approach for treatment of diseases such as prostate cancer (PC). The promise of siRNA-based therapeutics is dependent on the development of platforms that effectively protect siRNA from nuclease degradation and deliver the siRNA to the cytosol of target cells. The establishment of nanoparticle-based siRNA delivery platforms have been investigated to mitigate the cost and safety issues associated with viral delivery platforms. In this work, we present the development and characterization of a lipid coated mesoporous silica nanoparticle (LC-MSN) to address the need for safe and effective siRNA delivery across various biological barriers in the relapsed prostate cancer landscape. The LC-MSN utilizes calcium silicate nanogating over the silica core to efficiently load (80%) and release (>80%) siRNA in relevant media, as analyzed by tracking a fluorescently tagged siRNA cargo. Additionally, the calcium silicate core is encapsulated in a lipid bilayer aimed to improve the LC-MSN biocompatibility and enables the integration of GRP78 minibodies for targeted delivery to PC cells. The cytotoxicity, uptake and intracellular fate of the LC-MSN is investigated within our work using the LNCaP PC cell line. Furthermore, our work utilizes an ex ovo chick chorioallantoic membrane model (CAM) to assess LC-MSN system vascular margination, binding, circulation time and stability. The structural and chemical versatility of the silica nanoparticle core along with a biocompatible lipid coating makes the LC-MSN a promising candidate for siRNA delivery within the relapsed PC landscape.

G12 - Optimizing the Combination of Natural Pigments for Co-sensitization of Panchromatic TiO2 Dye Sensitized Solar Cells

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Six major classes of natural pigments (Anthocyanins, Betalins, Chlorophyll, Xanthonoids, Curcuminoids and Phycobilins) were explored in this work as potential sensitizers in Dye Sensitized Solar Cells (DSSC's) to replace expensive synthetic Ruthenium-containing dyes. Co-sensitization of natural dyes has been explored heavily in literature and has indicated symbiotic efficiency increases, however, no quantitative attempt has been made to optimize these combinations. Therefore, the goal of this work was to combine the six constituent dyes and produce so-called panchromatic solutions which closely matched the Air Mass 1.6 Global (AM1.5G) solar irradiance spectrum. UV/VIS absorbance data was collected for each individual dye as well as for every 1:1 and 1:1:1 molar combinations (a total of 42). Data was also collected for so-called "anode adsorbed" dyes which measured the absorbance profile of a transparent TiO2 anode which had been sensitized with a particular dye combination. This revealed the substantial differences in dye absorption associated with the TiO2 chelation process which greatly affected the panchromaticity. Therefore, distinctions between the data reference frame have been made in this work. Radial basis function interpolation was then used to generate surfaces mapping a six-dimensional real coordinate space to a one-dimensional real coordinate space ($R6 \rightarrow R1$) with precession through all measured UV/VIS data points. This allowed for the calculation of the resulting light harvesting efficiency (LHE) profile for any arbitrary dye combination using the data measured from the original 42 combinations. The LHE of a total of 2568 dye combinations were generated using this method which were then compared to the AM1.5G spectrum in one of three so-called "fitment conditions" designed to assess the commensurability between the two datasets. Therefore, a total of 6 optimized dye combinations were proposed corresponding to each fitment condition for both the bulk solution and anode adsorbed UV/VIS data regimes. DSSC's were then produced for each of the 42 original dye and 6 optimized combinations. An average efficiency of 0.29% was reported for all DSSC's with a standard deviation of 0.25%. The best performing optimized dye combination was generated from the anode adsorbed UV/VIS data and yielded an efficiency of 0.41%. However, the highest overall performing dye was a result of a 1:1 combination of Curcuminoids and α-Mangostin which yielded an efficiency of 1.31%. Co-adsorption of this dye combination with 1:1 Chenodeoxycholic acid (CDCA) yielded an efficiency of 1.54% which is the maximum efficiency reported in this work. While the optimized panchromatic dye solution did yield an efficiency ~1.5x greater than the statistical average, the performance of the Curcuminoids/α-Mangostin combination observed in this work suggests that panchromaticity alone is not sufficient to predict DSSC performance.

G13 - Synthesis and Functionalization of Barium Titanate Nanoparticles and Their Incorporation into Epoxy Composites

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Barium titanate (BTO) nanoparticles show great potential for use in electrostatic capacitors with high energy density. This includes both polymer composite and sintered capacitors. However, questions about the nanoparticles' size distribution, amount of agglomeration, and surface ligand effect on performance properties remain. Reducing particle agglomeration is a crucial step to understanding the properties of nanoscale particles, as agglomeration has significant effects on the composite dielectric constant. BTO surface functionalization using phosphonic acids is known reduce BTO nanoparticle agglomeration. We explore solution synthesized 10 nm BTO particles with tert-butylphosphonic acid ligands. These particles are then added to an epoxy matrix by desired volume percent, and the degree of agglomeration and capacitance are measured and examined. Finally, connections between degree of agglomeration, ligand interaction, device capacitance, and particle dielectric constant are made.

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G14 - Analysis of the effect of indentation spacing, specimen thickness and edge distance on the results of indentation tests

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Indentation hardness tests have wide-ranging application in engineering to obtain material hardness. In the current work, copper bars with different thicknesses were machined and grinded before indenting with a mechanically-instrumented Rockwell tester. Parameters including indentation spacing, specimen thickness and edge distance were studied for its effect on the hardness values. Moreover, 2D non-linear finite-element modelling was utilized to capture interaction between plastic zones lying beneath the indents. The simulation results showed competitive factors, the effect of material hardening owing to the plastic deformation induced by indentation and indent spacing, on the results of indentation tests.

G15 - Nanoscale magnetic imaging with nitrogen vacancy centers in diamond

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We used the photoionization dynamics of nitrogen vacancy (NV) centers in diamond to perform super-resolution magnetic microscopy with a resolution approaching 50 nm. We combined a donut-based super-resolution technique with optically detected magnetic resonance measurements on dense ensembles of NV centers to enable nanoscale magnetic imaging of ~30 nm iron-oxide nanoparticles.

Professional

P1 - Femtosecond Laser-based Machining of Small Scale Tensile Specimens

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We will introduce review recent developments in femtosecond laser-based machining of polycrystalline ceramic materials spanning from the micrometer to millimeter scale. The laser machining workstation features a 6 degree of freedom precision stage that is married to a galvanometer mirror that can be combined to mill microscale specimens from large scale ceramic parts. This system has been used for deep hole drilling in brittle materials and investigations of the feasibility of manufacturing micromechanical test specimens are underway. We will report previous results using a related method and machining system to understand the effects of intrinsic microstructural flaws in hot pressed SiC. In bulk specimens, microscale voids and inclusions dominate the tensile response and mask the role of the underlying microstructure. Microscale tensile bars were machined from SiC thin sections and subsequent tension tests showed that the fracture strength of microspecimens was dramatically higher than bulk tensile samples. An analysis of strength-size scaling suggested a transition in the dominant strength-determining flaw at the microscale. Analysis of fracture surfaces and critical flaw sizes suggest failure is governed by isolated large grains. The size-dependent strength variations have important implications for parameterizing ceramic failure models.

P2 - Redesigning Micro-Electromechanical Systems for Additive Manufacturing

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Micro-electromechanical systems (MEMS) are devices that sense and actuate at the microscale. Typically, MEMS devices are fabricated using multi-step, clean-room techniques which are time consuming in both design and fabrication and thus cost prohibitive for prototyping or small-scale production. Recently, simple MEMS actuators have been fabricated in a single-step approach using micro-scale 3D printing techniques such as multi-photon lithography (doi:10.1109/JMEMS.2020.2992367). Subsequent thin-film metal deposition produced dynamic MEMS that move through applied electrical power. In our work, we aim to adapt tried-and-true MEMS devices such as chevron actuators—traditionally fabricated using, for example, the SUMMiT V process developed at Sandia National Labs—to be compatible with additive manufacturing, and ultimately develop complex multicomponent systems and functions. The design for additive manufacturing approach (DfAM) employed here required many iterative design/test cycles to adapt planar, multi-level assemblies into more 3D free form fabricated objects. Following this iterative process, we demonstrate rotation of a 300-micron, 100-toothed gear via a linear thermal actuator coupled to a long-spanning cantilever. Overall, this work extends the capabilities and knowledge surrounding the use of microscale 3D printed structures for producing dynamic MEMS and has the potential to displace traditional microfabrication techniques that require dozens of process steps.

P3 - Integrating Blue Laser Manufacturing into LENS for Greater Material Flexibility

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1. Sandia National Laboratories

Traditionally, laser based additive manufacturing is done with 1064nm IR laser systems. These laser systems work well for many iron, titanium, and nickel based alloys but it can be difficult to print metals that are more reflective at that wavelength such as copper, gold, silver, and even aluminum. Because the more reflective metals are very thermally and electrically conductive, there is motivation to be able to print them in a fully dense state for various aerospace and defense applications. This poster will go over modifications that were made to the LENS (Laser Engineered Net Shaping) system at Sandia National Laboratories that allowed for an expanded suit of materials to be printed. This poster will also show and discuss initial metallurgical results from the system.

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P4 - Bonding of Bismuth Telluride Thermoelectrics with Lead-Borosilicate Glass

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Thermoelectric power generation modules utilize a "Seebeck Effect" to generate voltage when the module has a temperature differential on opposing surfaces. These modules are typically made of alternating N and P type bismuth telluride (BiTe) semiconductors bonded together with an epoxy. The epoxy acts as both a dielectric and thermal insulator between the N and P type BiTe. The epoxies can offgas and decompose at elevated temperatures resulting in temperature limitations of the module. Inorganic glasses with low softening point temperatures have the potential to replace epoxy and expand the use of these modules. The lead-borosilicate glass system is an ideal candidate for bonding BiTe as they can have softening points below 400 °C. A series of lead-borosilicate glass compositions with varying lead:boron ratios were batched, melted, and poured into ingots and characterized. The thermal expansion coefficient, glass transition temperature, and softening point were measured for the glass series. A clear trend for the lead content in the glass composition to measured properties was observed. The glass was machined into thin (<100 µm) sheets and used to bond the BiTe sheets. Results of the bonding process will be presented.

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P5 - Integrating atomic layer doping (ALDo) with CMOS circuitry for reduced contact resistance

Evan Anderson*[1]
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Leveraging atomic-scale control over material properties holds great promise for both reaching new levels of performance in existing devices and realizing new transistor technologies. Atomic Layer Doping (ALDo) uses surface chemistry to dope silicon at concentrations exceeding the solid solubility limit, but has traditionally been limited to laboratory-scale device fabrication with low throughput. Meanwhile, contact resistance is a large and increasing source of energy loss as contact areas decrease in modern transistors, with improvements in doping density offering a possible remedy. Here, we demonstrate doping densities far in excess of the state-of-the-art and present a process to insert ALDo into the middle of a CMOS flow, where contacts are often made. Electrical measurements of our multi-layer ALDo process shows an active density exceeding 1e21 dopants/cm3. We have developed an oxide hardmask using conventional photolithography enabling a path toward manufacturing patterned ALDo contacts and modified the ALDo process to start from a low-thermal-budget sputtering process. Thus, we have discovered a possible process for incorporating extreme concentrations of dopants and that are compatible with the middle-of-line for a CMOS process flow, enabling reduced contact resistance. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

P6 - Exploring iron nitride-based soft magnetic composites for electric vehicle technologies

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1. Sandia National Laboratories

Soft magnetic composites (SMCs) may improve the peak and specific power of electric motors while answering the need for cost reduction and replacement of rare earth materials. DOE 2025 goals target a peak power of 100 kW and a specific power of 50 kW/L in a motor operating at >20,000 rpm. This increased power needs to come at a cost of 3.3 $/kW. SMCs offer a low-cost alternative to rare earth permanent magnets. Conventional soft magnetic materials face decreased motor efficiency at high rotational speeds due to eddy current losses. However, SMCs feature an insulating matrix. The insulating matrix in SMCs may decrease eddy current losses and increase electrical resistivity enough to permit motors to operate with high efficiency at high rotational speeds. The authors' project work has explored iron nitride-based SMCs because γ'-Fe4N has a higher saturation magnetic polarization and electrical resistivity than silicon steel, a conventional soft magnetic material. The project entailed optimizing the chemistry, preparation, and cure of the iron nitride-based SMCs. Net-shaped iron nitride-based SMCs were prepared by curing in silicone molds. These materials were characterized by differential scanning calorimetry (DSC), scanning electron microscopy (SEM), magnetometry, thermal conductivity testing, and tensile testing.

P7 - Dry Electropolishing - A New Way to Prepare Metal Surfaces for Characterization

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Conventional electropolishing has its limitations, e.g., large temperature-controlled acid baths, corrosive liquids, greater amount of material removed during polishing, and large quantity of hazardous waste, to name a few. Recently a new technique known as “dry electropolishing” has emerged, which has advantages that allow for producing well-polished surfaces where it is conventionally difficult to achieve. This new capability has advantages in certain applications, particularly in the flexibility of materials it can polish, and the speed and quality to which it can polish specimens for characterization. Dry electropolishing has no temperature control needs. It combines tumble polishing and contact electropolishing by fixturing materials of interest to a holder that serves as the anode, which spins inside a humidity-wetted, highly crosslinked, polystyrene sulphonic acid bead media contained in a plated titanium net that serves as the cathode. The media preferentially polishes high frequency microscale features while reducing material removal at the macroscale. We have demonstrated successful utilization of the technique on a wide variety of materials such as, stainless-steel, Kovar, Inconel, Hiperco, aluminum, and titanium, needing only to optimize a handful of parameters to achieve the desired results. Furthermore, we have shown that it can be applied to traditional and additively manufactured samples of interest for microscopy characterization to improve polish (and by extension image quality) over mount-and-hand-polish methods, with orders of magnitude increases in throughput.

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P8 - Impedance Characteristics of Mo-SiNX and Mo-YSZ Granular Metals

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We present a study of the impedance response of granular metals (GMs), which are composites made of nanoscale metal islands dispersed in a dielectric matrix. These materials are unique such that the electrical transport below the percolation limit varies depending on the frequency regime.

In this study we synthesize GMs with Mo dispersed within an yttria-stabilized zirconia (YSZ) or SiNX insulator matrix. GMs are deposited with a target volumetric metal fraction (φ) from 0.2 to 0.8. GM impedance is measured from DC to 5 MHz, and from room temperature to 50 K. DC resistances are determined from current-voltage curves measured using a Van Der Pauw geometry at room temperature. High frequency responses as a function of temperature are measured using a parallel-bar electrode geometry. To qualify as a good high pass filter, the ratio of the DC to RF impedance must be several orders of magnitude. We find that low metal fraction samples, such as 20% Mo in SiNX, have ratios from 104-105. Selecting appropriate metal and insulator materials can optimize the overall impedance characteristics. Our results suggest that well-designed GMs have promise for high pass filter response applications. We will also discuss the development of the GM impedance measurements over many orders of magnitude.

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P9 - Thermomechanical Properties of Polyurea Nanocomposites Over Extreme Strain Rates

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Polyurea is commonly used as an encapsulant, a coating, and/or a binder to increase durability, corrosion, or impact resistance of surfaces. Unlike materials with similar chemistries, such as polyurethane, polyurea has a phase-separated microstructure consisting of hard-segments that are dispersed throughout a soft-segment matrix. This phase separation and hydrogen bonding in the material results in exceptional impact resistance and toughness, even at high strain rates and high strain levels. Here, we demonstrate enhanced thermal and mechanical properties of polyurea through the incorporation of nanoparticles. Surface modification of the nanoparticles was optimized to promote homogeneous particle dispersion, maximum particle volume fraction, and particle-matrix adhesion. Particle-matrix compatibility significantly affects the ultimate tensile stress for the nanocomposites. The dispersibility of particles is measured via rheology while the phase segregated microstructure and particle segregation is observed via atomic force microscopy. The mechanical performance of polyurea nanocomposites is compared to that of unfilled polyurea over an extreme range of strain rates (0.1-10,000 Hz) via dynamic mechanical analysis, Hopkinson bar, and shock tube testing, demonstrating the ability of polyurea nanocomposites to damp vibrational energies over a wide range of rates. Finally, highest strain rate insults were imposed in the Sandia National Laboratories SPHINX electron beam pulsed power facility, where the damping of mechanical energies of polyurea was measured to strain rates of 106 s-1 by imposing a thermomechanical shock in the material. Assessment of the damage to the polyurea as a result of electron beam radiation shows an exceptional resistance of the nanocomposites to radiation and thermal damage.

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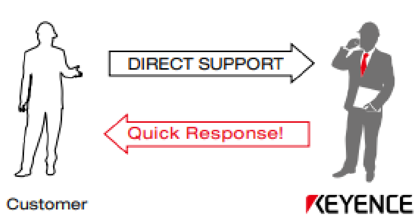

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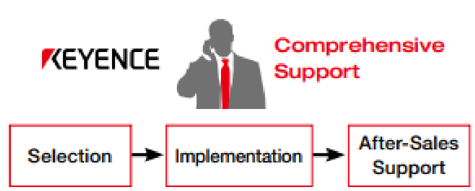

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