33rd Annual
Rio Grande Symposium on Advanced Materials

Held on October 23rd, 2023.

Oral Presentation Program Abstracts

Symposium Chair – Pankaj Kumar
Symposium Co-Chair – Elliott Fowler
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# Symposium Oral Presentation Program –

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Analysis of Defect Networks in Metamorphic Antimonides Grown on GaAs and Silicon using Transmission Electron Microscopy

Ganesh Balakrishnan\textsuperscript{1}, Fatih Ince\textsuperscript{1}, Mega Frost\textsuperscript{1}, Thomas Rotter\textsuperscript{1}, Darryl Shima\textsuperscript{1}

\textsuperscript{1}University of New Mexico, Albuquerque, NM

Speaker Name – Ganesh Balakrishnan  
**INVITED PRESENTATION**

Abstract –

Antimonide-based alloys have the capability to detect medium and long-wavelength infrared ranges of the EM spectrum. Furthermore, these structures can be realized on GaAs and Silicon substrates by using interfacial misfit dislocation (IMF) array growth mode and it has been shown that fully relaxed GaSb growth on GaAs with dislocation density of \~10 dislocations/cm is possible. In this presentation, it will be shown using transmission electron microscopy that further reduction of the dislocation density to \~10 is possible using AISb defect filter layers that bend dislocations due to the strain at the AISb/GaSb interface. In particular we will discuss the formation of a secondary network of dislocations at the AISb/GaSb interface that will allow for the annihilation of dislocations. In addition to the results on GaAs we will also discuss the growth of similar buffers on Silicon substrates.
**HF and UV/O3 Treatment for Reducing Leakage Current in GaN Schottky Barrier Diodes**

Amelia Peterson¹, Kim Kropka¹, Anthony Rice¹, Albert Colon¹, Greg Pickrell¹

¹Sandia National Laboratories, Albuquerque, NM

Speaker Name – Amelia Peterson

**Abstract –**

GaN Schottky barrier diodes have attracted attention due to their potential for use in high voltage, high power, and fast-switching applications. However, their performance can be dominated by surface states and edge effects leading to high leakage currents, premature breakdown voltages, and large ideality factors. Passivation treatments such as ion implantation or plasma treatments have been shown to mitigate these effects [1-2], but such treatments can also damage the lattice. To overcome these issues, we employ an HF wet etch followed by a low temperature ultraviolet light and ozone (UV/O3) treatment to etch and regrow a thin passivating Ga layer on the GaN surface around the anode. The electrical characteristics of a Pd-GaN diode are measured before and after the surface of the diode is treated with a 200C UV/O3 process, etched with HF, then treated with the same UV/O3 process again. This treatment resulted in a 21 times reduction in reverse bias current at -120V. These results demonstrate that this treatment is a potential alternative to high-energy or high-temperature processes for passivating leakage paths on GaN surfaces.

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


Tailoring Optics in Periodic Arrays Through Size-Dependent Lattice Resonances

Vahid Karimi\textsuperscript{1}, Viktoria Babicheva\textsuperscript{1}

\textsuperscript{1}ECE Department, University of New Mexico, Albuquerque, NM

Speaker Name – Vahid Karimi

Abstract –

Lattice resonances in metasurfaces arise from the constructive interference of electromagnetic waves with closely spaced subwavelength elements, inducing pronounced phase and amplitude responses. These resonances facilitate tailored control over light-matter interactions through precise modulation of the electromagnetic field distribution. Lattice resonances arise from synchronized electromagnetic wave oscillations in periodic particle arrays. These resonances are heavily influenced by particle size and inter-particle spacing, impacting device performance. Exploring size effects on lattice resonances in resonant particle arrays is vital for optimizing such systems. Array size, determined by particle count along each dimension, profoundly influences collective particle behavior and resulting resonances. Our study focuses on silicon and titanium antenna arrays, analyzing how altering the array period affects optical properties. Using coupled electric-magnetic dipole calculations, we find faster convergence in broad resonances for finite-size arrays. Our observations revealed that lattice resonances associated with higher-order diffraction (e.g., second-order) exhibited a more rapid convergence compared to those positioned adjacent to the first-order diffraction. Modifying the array period to adjust lattice resonances requires a larger array size for convergence.

Surface chemistry analysis of reworked GaAs substrates for i-line photoresist adhesion promotion for reworked wafers

Whitney Ingram¹, Clare Davis-Wheeler Chin¹, Carlos Sanchez¹, Tony Ohlhausen¹, Melissa Meyerson¹, Keith Fritzsching¹, William Corbin¹, Micah Murphy¹,
¹Sandia National Laboratories, Albuquerque, NM

Abstract –

This work describes a systematic comparison of GaAs wafer surfaces after various reworking processes to isolate photoresist adhesion failures, prevent failure propagating into downstream processing, and mitigate subsequent impacts on electrical device yields. GaAs (100) surfaces exposed photoresist were chemically cleaned with acetone, oxygen plasma, or n-methyl pyrrolidone (NMP). Effectiveness of organic material removal and impacts to GaAs bond structure and crystallinity were analyzed via SEM/EDS, TOF-SIMS, XPS, and XRD spectroscopy. Oxygen plasma most effectively removed residual resist-poisoning organic contaminants but generated an oxide layer the GaAs surface. I-V measurements of Schottky diodes prepared on reworked GaAs wafers were compared across all cleaning methods to assess device-level impacts. A detailed chemical analysis of NMP baths via NMR and mass spectrometry was also performed to assess impacts of suspected contaminants such as water, isopropanol, and NMP degradation products, and to elucidate mechanisms of adhesion interference. Results showed that NMP effectiveness for photoresist removal decreased with the introduction of contaminants. Overall, results indicate that residue left on wafer surfaces by insufficient cleans and chemical contaminants causes defects in the resist profile. To the best of the authors’ knowledge, this is the first reported study on the cleanliness of GaAs surfaces focused on photoresist adhesion issues re-worked wafers.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
**Frequency and Electric Field Dependent Conductivity of Mo-SiNX Granular Metals**

Michael McGarry¹, Simeon Gilbert¹, William Bachman¹, Luke Yates¹, Peter Sharma¹, Jack Flicker¹, Michael Siegal¹, Laura Biedermann¹

¹ Sandia National Laboratories, Albuquerque, NM

Speaker Name – Michael McGarry

**Abstract –**

Over the last ~50 years granular metal (GM) investigations have included fundamental scientific research (electron transport) and diverse applications (sensors, plasmonics). GMs are 3D structured composites, which comprise metal nanoparticles dispersed within an insulating matrix. By experimentally controlling the volumetric metal fraction (φ) and growth environment we can control the electrical properties. At low φ, the isolated nanoparticles exhibit electric-field (E-field) dependent electron tunneling transport (variable-range hopping, Poole-Frankel conduction, and Fowler-Nordheim tunneling) and frequency-dependent conductivity (σ), via capacitive transport. By rf co-sputtering Mo and SiNx in a partial N₂ growth environment, our team has created GMs with exceptional electrical response to E-field and frequency. With the high-dielectric strength SiNx, we were able to support E-fields up to 4 MV/cm, and routinely 1 MV/cm. These tests demonstrate all three E-field dependent transport mechanisms. The DC conductivity increases three decades as transport transitions from hopping to tunneling. We also demonstrate a strong σ response, with a seven order-of-magnitude increase in the AC conductivity from DC to 1 MHz. These properties may enable Mo-SiNx use in high-power shunt devices.

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.
**Multipole Resonance Control in High-Refractive-Index Antennas**  
Md Sakibul Islam¹, Viktoriia E. Babicheva¹  
¹Department of Electrical & Computer Engineering, MSC01, University of New Mexico,  
Albuquerque, NM  

Speaker Name – Md Sakibul Islam  

**Abstract** –  
High-refractive-index materials show an ability to manipulate light phase and amplitude when such scattering elements (or nanoantennas) are isolated or arranged in a cluster or array and form the so-called metasurface. To achieve this nanoscale manipulation of the incident light on a subwavelength scale, several metasurface parameters can be examined, for example, periodicity, aspect ratio, asymmetric effect, and oblique incidence. We design metasurfaces with multipole resonances in high-refractive-index antennas to show manipulation of incident light covering the ranges from visible to mid-infrared. Our analysis of asymmetric (truncated cone and cone) antennas shows an accidental bound state in the continuum (BIC) due to vanishing resonance linewidth in the infrared region. In a rectangular lattice array, we show that changing periodicity shifts the spectral position of resonance by moving it along the Rayleigh anomaly. We show asymmetric antennas transform overlapping between electric dipole and magnetic dipole resonances as Kerker effect into coupling between them as Rabi splitting. We show excitation of an out-of-plane magnetic dipole resonance for small changes in oblique incidence and enhancement of symmetry-protected BIC as resonance linewidth collapse at normal incidence. The transformation of the symmetric antenna (disk) into an asymmetric (cone) antenna confirms the enhancement of resonance in the intermediate asymmetric (truncated cone) shape.
How Spatially Resolved Mechanical Testing Can Help Inform Weld Process Development

Priya Pathare\textsuperscript{1}, Christopher Finfrock\textsuperscript{1}, Jeffrey Rodelas\textsuperscript{1}, Jay Carroll\textsuperscript{1}
\textsuperscript{1}Sandia National Laboratories, Albuquerque, NM

Speaker Name – Priya Pathare

Abstract –

Understanding the strength of welded metal joints is crucial for designing safe engineering structures. However, because of the complex chemical and microstructural changes that occur during weld processing, it is impossible to predict weld performance using the vendor-supplied datasheet properties of the base metal and filler metal alone. For this reason, spatially resolved mechanical testing of the weld is needed. In this work, we extract mechanical properties found in the base metal, heat affected zone, and weld metal of hybrid-laser arc welds (HLAW) to inform decisions about weld process and heat treatment selection. Mechanical properties along various positions in a narrow groove multipass HLAW are assessed using digital image correlation and clever sample fabrication. This approach revealed the underlying processing-property relationships that can be used to achieve peak performance combinations during welding process development.

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Joining Al2O3 to Kovar via Zirconium Active Braze: Dynamic Investigation with In-Situ Video Monitoring

Anthony McMaster¹, Pankaj Kumar², Jessica Kopatz¹, Patrick Price¹, Ed Arata¹
¹ Sandia National Laboratories, Albuquerque, NM
² University of New Mexico, Albuquerque, NM

Speaker Name – Anthony McMaster

Abstract –

Brazing is one of the few available methods for producing hermetic, high strength joints between ceramic materials and metals. Active brazing allows the joining to occur in a single step through a metallization reaction at the ceramic-braze alloy interface. Here, video monitoring was implemented to determine reaction stages, time and length scales, and causes of failure for an AgCuZr braze alloy joining Al2O3 to Kovar. The collected video data was correlated to postmortem analysis of SEM and EDS (energy-dispersive X-ray spectroscopy) to quantify elemental transport. In situ monitoring provides new insight into the reactions that occur in active braze joining, especially at the interface between the braze alloy and ceramic substrate.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
Improved Throughput Exploration of Electrolyte Species: A Study of Chelating Agents and pH in Metal Film Electrodeposition

Lauren Bailey¹, Jonathan Coleman¹,
¹ Sandia National Laboratories

Speaker Name – Lauren Bailey

Abstract –

Electrodeposition is an incredibly capable yet equivalently complex process to synthesize materials and coatings. To take advantage of machine learning statistical analysis tools and COTS automated instruments, we developed a strategy and process to study variable complexing agents and pH electrolyte systems for the controlled synthesis of metal films. In this study we utilized an optimized method of solution making, which relied on an automated micropipetter, allowing us to efficiently produce an array of solutions with pHs varying from 1-13. This procedure allowed us to observe the metal precursor solubility based on pH, depending on complexing agents. The information learned from these studies were used to coordinate the solutions we would use for deposition and the method to produce them. We also varied the current densities used while plating across a range of pH. Optical Microscopy was used to characterize the plated tokens and investigate the influence pH has on the viability of an electrolyte to function for electrodeposition. Our data explores opportunities for optimizing the electrodeposition process, enabling development of novel metal films with tailored properties by interpolating and extrapolating apparent trends. The insight from this study shows the vital role that the complexing agents and the pH of a solution have in electrodeposition, and how we may take advantage of increased exploration.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
Manufacturing of Refractory complex concentrated alloy by Powder Metallurgy

Surya Bijjala¹, Pankaj Kumar¹

¹ Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131

Speaker Name – Surya Bijjala

Abstract –

Refractory complex concentrated alloys (RCCAs) are considered as the next generation high temperature (HT) materials due to their superior high temperature properties over conventional alloys. In particular, NbMoTaWVRCCAs are considered to be the potential candidate due to their promising HT stability and mechanical properties. However, these alloys suffer from poor room temperature (RT) ductility which limits their practical application. Alloying with titanium has shown to improve the RT ductility without significantly reducing the HT strength. We studied manufacturing potential of NbMoTaWVTiRCCAs with x = 2, 8, 16, 27 at. % by powder metallurgy (PM) techniques, pressureless sintering, hot-isostatic pressing (HIP) and spark plasma sintering (SPS). All the PM techniques yielded high density RCCAs. A Ti rich phase was precipitated in the microstructure in all RCCAs compositions irrespective of the manufacturing techniques. Preferential segregation of oxygen to the Ti rich phase was observed. The volume fraction of precipitated phase was observed to increase with the increase in Ti content in RCCAs.
Solder Joint Reliability in Fine Pitch Ball Grid Arrays
Jessica Buckner¹, Jeier Yang¹, Scott Bobbit¹, Rebecca Wheeling²

¹ Sandia National Laboratories, Albuquerque, NM, 87123
² Medtronic, Minneapolis, MN, 55432

Speaker Name – Jessica Buckner

Abstract –

Commercial-off-the-shelf ball grid array packaging technologies are trending towards smaller pitch sizes. As pitch size decreases, metallurgical interactions occurring along the interface may begin to dominate the mechanical behavior of the joints due to solder volume per joint decreasing. Furthermore, it is unknown whether the current solder fatigue model breaks down for solder ball interconnects as size decreases. This work aims to provide empirical validation of solder joint reliability for 0.40, 0.65 and 0.80 mm solder pitch sizes for both SAC305 and Sn63Pb37 alloys. Isothermal aging of the boards was performed to understand the kinetics of intermetallic formation at the interface and microstructural evolution, then compared to density functional theory potentials. Thermal cycling (-55 °C/125 °C) was performed on assembled test boards. Shear testing and cross-sectional characterization were performed post-cycling to determine crack formation and failure behavior. The results are discussed in the context of pitch size effects and intermetallic formation.

Sandia National Laboratories is a multimission Laboratory managed and operated by National Technology Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy National Nuclear Security Administration under contract DE-NA0003525.
Highly Stable Fe and Ca codoped Barium Niobate Based Electrocatalysts for Effective Electrochemical Coupling of Methane to Ethylene

Kannan Ramaiyan, Luke Denoyer, Angelica Benavidez, Fernando Garzon,

Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM 87131, USA.

Speaker Name – Kannan Ramaiyan

Abstract –

Methane conversion into value-added products such as olefins and aromatics is gaining increased attention in the wake of new natural gas reserve discoveries. Electrochemical oxidative coupling of methane (E-OCM) provides better product selectivity as the product distribution can be controlled by applied potential as well as the oxide ion flux. Here a new catalyst based on Ca and Fe codoped barium niobate perovskites is reported for E-OCM electrocatalysts. These doped niobates showed enhanced thermochemical stability in SOFC-relevant conditions and catalytic activity towards methane activation. The redox behavior of the couple seems to be a key reason behind this redox stability while the size and electronegativity of the dopants affect the electrical properties. The chemical stability was analyzed by TGA measurements followed by analysis of the perovskite powders using PXRD measurements. Impedance measurements were utilized to analyze their electrical conductivity. Our results demonstrate doped barium niobates as a promising candidate for stable operation in high-temperature electrochemical applications.


L. H. Denoyer, A. Benavidez, A. Brearley, K. Ramaiyan, F. H. Garzon, Chemical Stability of BaMg0.33Nb0.67-XFeXO3 in High Temperature Methane Conversion Environments, ECS Transactions 2023, 111, 587.

L. H. Denoyer, A. Benavidez, F. H. Garzon, K. P. Ramaiyan, Chemical Stability of BaMg in High-Temperature Methane Conversion Environments; Energy Fuels, Under Revision.

L. H. Denoyer, A. Benavidez, F. H. Garzon, K. P. Ramaiyan, Highly Stable Doped Barium Niobate Based Electrocatalysts for Effective Electrochemical Coupling of Methane to Ethylene, Advanced Materials Interfaces, 2200796 (1-9)
**Materials Development and Testing for Extreme Environments**

Osman Anderoglu\textsuperscript{1}, Madhavan Radhakrishnan\textsuperscript{1,2}, Xiatong Yang\textsuperscript{1}, Nathan Mara\textsuperscript{3}, Justin Cheng\textsuperscript{3}, Thomas Nizolek\textsuperscript{4}

\textsuperscript{1} Department of Nuclear Engineering, University of New Mexico
\textsuperscript{2} University of North Texas
\textsuperscript{3} University of Minnesota
\textsuperscript{4} Los Alamos National Laboratory

Speaker Name – Osman Anderoglu

**INVITED PRESENTATION**

**Abstract** –

Structural materials for advanced Generation IV nuclear reactors are expected to withstand extreme environments including elevated temperatures up to 1000°C and irradiation doses more than 200 displacement per atom (dpa) while in contact with very corrosive coolants such as heavy liquid metals. Recent results on nanolayered composites have proven to be a very promising approach that can address the requirements for advanced reactors with careful selection of constituting materials. In these alloys, the interfaces act as obstacles to dislocation motion and sinks for irradiation induced point defects. As a result, a high-volume fraction of interfaces provide over an order of magnitude strength and remarkable irradiation resistance compared to single phase counterparts. In this presentation, I will talk about stability of nanolayered composites under heavy ion irradiation. While Cu/Nb shows remarkable stability at very high irradiation doses, Zr/Nb loses layered morphology completely. Although both systems are immiscible at selected irradiation temperature, thermal spikes thought to be cause of layer mixing. Stronger de-mixing forces in Cu/Nb lead to layer separation during thermal spikes.
**Fabrication, Thermal Analysis, and Heavy Ion Irradiation Resistance Epoxy Matrices with Silane-Capped Ceria Nanoparticle**

Clare Davis-Wheeler Chin\(^1\), Marissa A. Ringgold\(^2\), Erica M. Redline\(^4\), Avi G. Bregman\(^2\), Khalid Hattar\(^3\), Amanda S. Peretti\(^4\), LaRico J. Treadwell\(^2\)

\(^1\) Microsystems and Engineering Sciences Applications Complex, Sandia National Laboratories
\(^2\) Advanced Materials Laboratory, Sandia National Laboratories
\(^3\) Ion Beam Laboratory, Sandia National Laboratories
\(^4\) Sandia National Laboratories

Speaker Name – Clare Davis-Wheeler Chin

**Abstract** –

This work describes a detailed understanding of how nanofillers function as radiation barriers within the polymer matrix, and how their effectiveness is impacted by factors such as composition, size, loading, surface chemistry, and dispersion. We designed a comprehensive investigation of heavy ion irradiation resistance in epoxy matrix composites loaded with surface-modified ceria nanofillers, utilizing tandem computational and experimental methods to elucidate radiolytic damage processes and relate them to chemical and structural changes observed through thermal analysis, vibrational spectroscopy, and electron microscopy. A detailed mechanistic examination supported by FTIR spectroscopy data identified the bisphenol A moiety as a primary target for degradation reactions. Results of computational modeling by the Stopping Range of Ions in Matter (SRIM) Monte Carlo simulation were in good agreement with damage analysis from surface and cross-sectional SEM imaging. All metrics indicated that ceria nanofillers reduce the damage area in polymer nanocomposites, and that nanofiller loading and homogeneity of dispersion are key to effective damage prevention. The results of this study represent a significant pathway for engineered irradiation tolerance in a diverse array of polymer nanocomposite materials. Numerous areas of materials science can benefit from utilizing this facile and effective method to extend the reliability of polymer materials.
Effects of Heat Treatment Under External Magnetic Field on Microstructure of Ferritic/Martensitic Steels

Xiatong Yang¹, Kirk Lemmen², Keaton Looper², Nan Li³, Stuart Maloy⁴, Haluk Karaca², Osman Anderoglu¹

¹ Department of Nuclear Engineering, University of New Mexico, Albuquerque, NM 87131
² Department of Mechanical Engineering, University of Kentucky, Lexington, KY 40506
³ Los Alamos National Lab, Los Alamos, NM 87544
⁴ Pacific Northwest National Lab, Richland, WA 99352

Speaker Name – Xiatong Yang

Abstract –

Ferritic/Martensitic steels are among the most promising candidates for structural and cladding applications in advanced reactors because of their excellent thermal properties and swelling resistance compared to conventional austenitic stainless steels [1]. However, there F/M steels still suffer from radiation embrittlement at low temperatures, creep at higher temperatures and swelling at very high irradiation dose at intermediate temperatures (400-450°C) [2,3]. Heat treatment under external magnetic field can potentially address some of these challenges. Tempering under magnetic field could change the interfacial energy of carbon precipitates thus altering the morphology and distribution of carbides [4]. The spheroidization of carbides could help reduce the sharp corners which is the concentration point of stress to improve the mechanical behavior [5]. The finer distribution of carbides on the sub-grain boundary could help hinder the gliding of dislocations thus increasing the creep resistance. Lath spacing can also be optimized to increase volume fraction of interfaces [6]. Together with smaller precipitates, these interfaces can provide recombination sites for radiation induced point defects resulting in improved resistance. In this talk, I will present an overview of the magnetic field heat treatment effects on F/M steels together with our recent progress.
Metallographic Characterization of Oxidation Behavior in Tantalum and its Alloys

Michael Rene Lopez-Duran\textsuperscript{1,2}, James Whitaker\textsuperscript{1}, Christian Harris\textsuperscript{2}, Zahra Ghanbari\textsuperscript{1}, Christopher Finfrock\textsuperscript{1}, Haluk Karaca\textsuperscript{2}, Osman Anderoglu\textsuperscript{1}

\textsuperscript{1} Sandia National Laboratories, Albuquerque, NM
\textsuperscript{2} The University of Texas At El Paso, El Paso, TX

Speaker Name – Michael Rene Lopez-Duran

Abstract –

Tantalum and its alloys are prone to oxygen embrittlement at moderate to high temperatures. The process is not fully understood due to uncertainties in the oxidation kinetics of the refractory material. Fundamentally understanding this behavior at temperatures ranging from 200 to 700 °C proves difficult while ensuring no further uptake of oxygen occurs on the metallographically prepared surface. This study, which used standard metallographic processes as a benchmark, attempted to improve and understand surface preparation techniques while also conducting microhardness measurements to experimentally resolve oxygen uptake. The metallographic preparation process developed through this work allows for clearer observations of microstructure evolution and microhardness, as well as quantitative assessments of oxygen content that are slated to occur in ongoing work.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
**Novel Tamper-Indicating Materials**

Cody Corbin\(^1\), Stephanie White\(^1\), Clayton Curtis\(^1\), Corey Parada\(^3\), Matt Humphries\(^3\), Hiedi Smartt\(^4\)

\(^1\) Sandia National Laboratories

Speaker Name – Cody Corbin

**INVITED PRESENTATION**

**Abstract** –

Tamper-indicating materials that dramatically and irreversibly transform color upon physical damage are important for a variety of applications. These materials are akin to permanently bruised skin. A multidisciplinary team at Sandia National Laboratories has developed different material sets with properties that 1) show a visible and dramatic color change, 2) involve chemistry/materials that are difficult to counterfeit and repair, and 3) have unique identification features. Initial attempts focused on polymer systems in which a bi- or tridentate -donor ligands, such as 2,6-bis(1-methyl-1-benzoimidazol-2-yl)-4-pyridinol, were incorporated into the chemical backbone. Chelation and colorimetric studies with transition metal ions was evaluated for tamper-indicating use as a homogenous composite system. Next, a different approach was taken using L-3,4-dihydroxyphenylalanine (L-DOPA), an O reactive species, as the colorimetric indicator in a thermoset material system. Targets, processing challenges, and results of work will be discussed in detail.

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.
Rational Design of Silica Nanoparticles for Overcoming Barriers of siRNA Delivery in Relapsed Prostate Cancer Applications

Angelea Maestas-Olguin¹, Achraf Noureddine¹
¹UNM Chemical and Biological Engineering

Speaker Name – Angelea Maestas-Olguin

Abstract –

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 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.
The Recycling of Polybutadiene Rubber with Tunable Thermal Depolymerization Enabled by Microencapsulated Metathesis Catalysts

Matt Warner¹, Mikayla Romero¹,², Brad Jones¹

¹ Sandia National Laboratory
² University of New Mexico

Abstract –

The effective management of plastic waste streams to prevent plastic land and water pollution is a growing problem that is also one of the most important technological, political, and economical challenges facing plastic materials today. To achieve this, it is desirable to manufacture polymer materials that are both stable over their intended lifetime and easy to cheaply recycle or repurpose them as desired. However, achieving both satisfactory stability and recyclability is difficult for many commodity plastics. It is especially difficult to conceive this with crosslinked polymers such as rubbers because they cannot be molten and reprocessed in that manner. In this work, we explore the possibility for the depolymerization and reprocessing of polybutadiene (PB) rubber using microencapsulated Grubbs catalysts. Second-generation Hoveyda-Grubbs catalyst (HG2) contained within glassy thermoplastic microspheres can be dispersed in PB rubber below the microsphere glass transition temperature (Tg) without adverse depolymerization, evidenced by rubber with and without these microspheres obtaining a somewhat similar shear storage modulus of 16 and 28 kPa respectively. The thermoplastic Tg can be used to tune the depolymerization temperature, via release of HG2 into the rubber matrix. For example, using poly(lactic acid) vs polysulfone results in a depolymerization temperature of 85°C and 162°C respectively. Liquefaction of rubber to a mixture of small molecules and oligomers is demonstrated using only a 0.01 mol% catalyst loading using poly(lactic acid) as the encapsulant. At that same catalyst loading, depolymerization occurs to a greater extent in comparison to two ex-situ approaches, including a conventional solvent-assisted method, where it occurs at roughly twice the extent at each given catalyst loading. In addition, depolymerization of the microsphere-loaded rubbers was demonstrated for samples stored under nitrogen for 23 days. Lastly, we show that the depolymerized products can be reprocessed back into solid rubber with similar mechanical properties. Henceforth, we envision that this approach could be used to recycle and reuse crosslinked rubbers at the end of their product lifetime and divert it away from plastic waste streams.
Polydiacetylenes: A Suite of Security
Cody Corbin¹, Stephanie White¹, Clayton Curtis¹, Heidi Smartt¹
¹ Sandia National Laboratories

Speaker Name – Cody Corbin

Abstract –

Treaty verification regimes rely on tamper-indicating technologies to maintain continuity of knowledge in between inspections. These technologies must indicate that tamper into equipment other items of interest has occurred and indicate evidence of attempted repair. The R&D that will be discussed revolves around specific colorimetric details of polydiacetylenes (PDA) and their response to multiple stimuli, including thermal, mechanical, chemical, and electrical attack vectors. Interactions with neighboring headgroups, and how those headgroups interact with other molecules during solvent-based attacks, dictate the color response and reversibility. Literature has shown how specific PDAs react for some types of stimuli, but no R&D has been performed evaluating how a PDA responds to all types of stimuli, which could be utilized for improved tamper indication. At a qualitative level one could easily differentiate an attacked PDA system from an intact version due to the blue-to-red transition. The quantitative color change would be verified via RBG analysis post-mortem to better understand the attack methodology. This talk will detail the progress on this endeavor.

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**Fuel Cell Component Durability for Million Mile Fuel Cell Trucks**

Rod Borup¹, Adam Weber², Deborah Myers³, K.C. Neyerlin⁴, Ahmet Kusoglu², Rajesh Ahluwalia³, Rangachary Mukundan², David Cullen⁵, and Jacob Spendelow¹

¹ Los Alamos National Laboratory (LANL), Los Alamos, NM
² Lawrence Berkeley National Laboratory (LBNL), Berkeley, CA
³ Argonne National Laboratory (ANL), Lemont, IL
⁴ National Renewable Energy Laboratory (NREL), Golden, CO
⁵ Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

Speaker Name – Rod Borup

**INVITED PRESENTATION**

**Abstract –**

While significant advances have been made and early commercial fuel cell light-duty vehicles (LDVs) are starting to be produced, fuel cells in the heavy-duty-vehicle (HDV) transportation sector (including trucks, long-haul semitrailers, maritime, trains, etc.) are nascent, despite the fact that advantages of fuel cells compared to both diesel and electric powertrains are very compelling in terms of emissions, charging time, efficiency, power-to-weight ratio, among others. However, the fuel-cell technology for HDVs requires a paradigm shift in fuel-cell research and development compared to LDVs, where the emphasis becomes efficiency and improvements in durability instead of a focus on increased power densities and lower cell costs. Heavy-duty applications require significantly longer vehicle lifetimes (>25,000 hours/1,000,000 miles for heavy-duty trucks), and therefore require improved fuel cell durability compared to light-duty vehicles.

To advance performance and durability of polymer electrolyte membrane fuel cells (PEMFCs), the M2FCT (Million Mile Fuel Cell Truck) consortium was formed; Los Alamos National Lab co-leads this consortium. M2FCT is an integrated consortium that includes: (i) modeling analysis to define drive cycles, operating conditions and requirements, (ii) material development for design/synthesis of durable high-performing materials based on previously developed materials, (iii) integrating these materials into MEAs (Membrane Electrode Assemblies), testing and modeling of material performance and enabling their scale-up and manufacturing, and (iv) accelerated stress test (AST) development and durability evaluation to enable these MEAs and materials to meet the efficiency/durability targets.

**Acknowledgments**

This work was funded through the DOE M2FCT Consortium with thanks to DOE EERE HFTO, Fuel Cell Technologies Office. Team Leader: Dimitrios Papageoropoulos and Technical Development Manager: Greg Kleen.
Enhancing Robustness of Fuel Cell Electrodes via Pt Thin Film Catalysts

Wipula Liyanage\textsuperscript{1}, Siddharth Komini Babu\textsuperscript{1}, Alper C. Ince\textsuperscript{1}, Jacob S. Spendelow\textsuperscript{1}, Rod Borup\textsuperscript{1}

\textsuperscript{1}Los Alamos National Laboratory, Los Alamos, NM

Abstract –

In recent years, there has been a growing interest in polymer electrolyte membrane fuel cells (PEMFCs) owing to their impressive attributes, including high power density, exceptional energy efficiency, and the eco-friendly advantage of zero emissions. These qualities position PEMFC-powered fuel cell electric vehicles (FCEVs) as game-changers in the quest to significantly reduce carbon dioxide emissions in the transportation sector, thus facilitating the widespread adoption of the hydrogen economy. However, to make this vision a reality, it is imperative to enhance the durability and resilience of fuel cell systems before FCEVs can be commercially viable on a broader scale. In this study, we introduce an innovative materials strategy aimed at mitigating cell damage. We achieve this by employing a thin film Pt anode catalyst supported on Nafion nanowires in a co-axial configuration. The use of Nafion nanowires with their high roughness eliminates the necessity for traditional carbon support, resulting in outstanding resilience against support corrosion, catalyst corrosion, and anode reversal. This research comprehensively evaluates the effectiveness of Coaxial Nanowire Electrodes (CANE) as both fuel cell cathodes and anodes with reversal tolerance, comparing their performance to conventional supported catalysts (Pt/C).
**Effect of the EMIM Cation on the CO2 Reduction Reaction on Gold**

Danielle Richards¹, Stephen J. Percival¹

¹ Sandia National Laboratory

Speaker Name – Danielle Richards

**Abstract –**

The electrochemical CO2 reduction reaction (CO2RR) is emerging as a promising method to produce carbon neutral chemical feedstocks. Additives or co-catalysts in the electrolyte can lower the activation barrier for CO2RR, yielding faster conversion rates at lower voltages. Recently, electrocatalytic CO2 reduction mediated by ionic liquids (IL) has been reported but with conflicting accounts to whether the ILs benefit CO2RR or adversely, the competing hydrogen evolution reaction (HER). We report the effect of added IL EMIM-Cl, specifically EMIM in aqueous solutions on the electrochemical CO2RR and competing HER on gold. We show the CO2 reduction current increases by ~1.5x with the highest amount of added EMIM relative to the pure electrolyte. Differential pulse voltammetry reveals an additional large change in the reduction current that only appears with both CO2 and EMIM present. Lastly, we use advanced electrochemical analysis methods to determine the reaction kinetics and preliminary evidence shows that the standard heterogeneous rate constant increases for the reaction at large overpotentials while the HER is suppressed at low overpotentials with EMIM present.

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Durability Study of Titanium-Supported Iridium (Ir/Ti) Anode Catalysts in PEM Water Electrolyzers

Kui Li¹, Xiaojing Wang¹, Rangachary Mukundan², Jacob S. Spendelow¹, Siddharth Komini Babu¹

¹ MPA-11: Material Physics and Application, Los Alamos National Laboratory, Los Alamos, NM, USA
² Lawrence Berkeley National Laboratory

Speaker Name – Kui Li

Abstract –

Electrochemical water splitting has been recognized as one of the most promising methods for hydrogen production. Electrocatalysts are critical materials in water electrolysis. The sluggish reaction kinetics for the anode reaction, oxygen evolution reaction (OER), hinders the development of water electrolysis technology. Iridium-based material is an leading catalyst for OERs, but the high scarcity and high cost limit its application in polymer electrolyte membrane water electrolyzers (PEMWEs). Moreover, Ir dissolution during the OER operation is another limitation. Robust and effective support-based catalysts should be developed to reduce the catalyst loading and provide high durability in PEMWEs. Herein, we synthesized an OER catalyst of Ir deposited on Ti supports using a polyol reduction method. The Ir/Ti catalysts with different Ir loading were prepared and applied in the PEMWEs for performance evaluation. The cell performance (Figure 1A) with the optimized catalyst (Ir/Ti-50%Ir) exhibited better performance than the commercial IrO. Accelerated stress tests (ASTs) performed between 2.0 V and 1.45 V were used to investigate the catalyst durability in the PEMWEs. Figure 1B shows a volcano shape for the correlation between degradation behavior and Ir percent in the catalyst. Our results, combined with the characterization, provide a synthesis strategy for robust OER catalysts, and elucidate the catalyst degradation mechanism in the PEMWEs.
Compensating for Sintering Distortion in Additively Manufactured Copper using Physics-Informed Gaussian Process Regression

Samuel Moran¹, Annika Bauman¹,²
¹ Sandia National Laboratories
² New Mexico Tech

Speaker Name – Samuel Moran

Abstract –

Copper is a challenging material to process using laser-based additive manufacturing due to its high reflectivity and high thermal conductivity. Sintering-based processes can produce solid copper parts without the processing challenges and defects associated with laser melting; however, sintering can also cause distortion in copper parts, especially those with thin walls. In this study, we use physics-informed Gaussian process regression to predict and compensate for sintering distortion in thin-walled copper parts produced using a Markforged Metal X bound powder extrusion (BPE) additive manufacturing system. Through experimental characterization and computational simulation of copper viscoelastic sintering behavior, we can predict sintering deformation. We can then manufacture, simulate, and test parts with various compensation scaling factors to inform Gaussian process regression and predict a compensated as-printed (pre-sintered) part geometry that produces the desired final (post-sintered) part.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
**Corrosion Susceptibility of LPBF 316L Stainless Steel in a Constant Contamination Environment**

Kasandra Escarcega Herrera\textsuperscript{1,2}, Michael Melia\textsuperscript{1}, Peter Renner\textsuperscript{1}

\textsuperscript{1} Sandia National Laboratories, Albuquerque, NM

\textsuperscript{2} The University of New Mexico, Albuquerque, NM

Speaker Name – Kasandra Escarcega Herrera

**Abstract –**

Laser powder bed fusion (LPBF) is a relatively new manufacturing technique capable of creating complex metal components. However, LPBF produces alloys with tortuous surfaces which can degrade corrosion resistance when compared to their wrought counterparts. As a result, as-printed (AP) LPBF surfaces are often treated through mechanical polishing (MP) or electropolishing (EP). This study compares the corrosion susceptibility of 316L stainless steel made by traditional and LPBF processes. Samples were exposed to a constant contamination and environment (300 $\mu$g/cm\textsuperscript{2} artificial sea water (ASW) salt loading, 40\%RH, 35°C) for 12 months. A characterization process was developed involving optical and scanning electron microscope (SEM) imaging to assess site specific corrosion. These images were used to quantify and compare corrosion site density across AP and polished surfaces. This process revealed the most common initiation site for corrosion to be along melt track boundaries which was verified by cutting into the samples with focused ion beam. This indicated the easiest propagation pathway was along melt pool boundaries. Electrochemical properties of AP, wrought, and polished 316L LPBF surfaces under full immersion conditions with ASW solutions were examined to corroborate the exposure results.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003524.
**Photothermal effects of plasmonic nanoparticles to enhance Diels-Alder (DA) reactions in reversible thermosets**

Arnob Dipta Saha\(^1\), Brandon T. McReynolds\(^2\), Madeline Finale\(^1\), Julio Cubillas\(^1\), Dr. Youngmin Lee\(^1\), John McCoy\(^2\), Sanchari Chowdhury\(^1\)

\(^1\) Department of Chemical Engineering, New Mexico Tech

\(^2\) Department of Materials and Metallurgical Engineering, New Mexico Tech

Speaker Name – Arnob Dipta Saha

**Abstract** –

Thermosets excellent mechanical properties, chemical resistance, and thermal stability make them an appealing material for additive manufacturing. Irreversible crosslinking and slow curing rate of thermosets like epoxy, however, makes layer by layer printing difficult. We have developed a reversible thermosets polymer incorporating thermo-reversible covalent adaptable network (Diels-Alder (DA) reactions) into it and mixing that with refractory plasmonic titanium nitride (TiN) nanomaterials. TiN nanoparticles can efficiently, rapidly convert broad spectrum visible light into localized heating to trigger rapid polymerization and depolymerization reactions making them suitable for reprocessing as well as additive manufacturing. Additionally, it provides opportunity for targeted repair of defect on a 3-D printed epoxy structure and smoothing the rough surface of the finished products. In this study, a comparative investigation was conducted between heat and light stimulus to examine their effect on Diels-Alder reactions. Our in-situ FTIR study of reversible epoxy/TiN composites under light suggested that broad spectrum white light can significantly enhance the reversible reactions. Interestingly, the reaction rate with light is significantly faster than the reaction driven by heat even though the average bulk temperature of the samples is similar. Plasmonic TiN nanostructures concentrate incident light in nanometer-sized volumes to generate nanoscale heating which cause the local temperature around nanoparticles hotter than the bulk temperature measured. Moreover, optical microscopy and atomic force microscopy images demonstrate that we can use light to precisely depolymerize a selected surface region of manufactured items to smooth out their rough surfaces or repair any cracks.
First-principles-derived flexible polarizable force fields for metal-organic frameworks for helium purification applications

Alma C Escobosa¹, Reza Ghanavati¹, Thomas A. Manz¹

¹ New Mexico State University

Abstract –

Helium has been in short supply for several years. To expand the helium supply, new routes to purify helium from natural gas sources should be explored. Because current helium purification processes are energy intensive, it is useful to explore alternate purification processes, such as membranes, that could potentially lower the energy requirements. Mixed matrix membranes that contain metal-organic framework (MOF) nanocrystals embedded in a continuous polymer matrix can have higher selectivities and permeabilities than pure polymer membranes. MOFs are characterized by their large surface areas as well as their tunable and flexible structures. Since there are endless organic linker/metal center combinations to form MOFs, computational screening is helpful to identify which particular MOF structures are best suited for a chosen target application. Molecular simulations require force fields (interatomic potentials) to generate an accurate computational representation of a MOF. In this work, we develop force fields that are simultaneously polarizable and flexible. These flexible polarizable force fields contain both non-bonded and bonded contributions to the potential energy. We developed a protocol to create flexible polarizable force fields for MOFs using data from density functional theory (DFT) calculations to extract the parameters needed in the force field. We are using these force fields in classical molecular dynamics and Monte Carlo simulations to compute the adsorption and diffusion properties of helium, methane, and N gases in MOFs. We use this data to estimate gas selectivities and permeabilities through the MOF and then through mixed matrix membranes. Finally, we construct process flow diagrams to purify helium from natural gas using these mixed matrix membranes.


**Influence of Precursor Design on Formation of a Reversible Diels-Alder Network**

Gaeun Kim¹, Brandon T. McReynolds², Samantha Knight¹, Nicole Penners¹, Sanchari Chowdhury¹, John McCoy², Youngmin Lee¹

¹ Department of Chemical Engineering, New Mexico Institute of Mining and Technology
² Department of Materials and Metallurgical Engineering, New Mexico Institute of Mining and Technology

Speaker Name – Gaeun Kim

**Abstract –**

Diels-Alder (DA) chemistry can be used to synthesize 3D printing thermosets that are capable of recycling and self-healing due to its ability to form networks at low temperatures and dissociate at high temperatures. Similar to conventional thermosets that need additional curing steps to achieve full mechanical strength, reversible thermosets also require a post-curing step upon printing. A long post-curing step can become a limitation as it can increase the processing time and potentially alter the dimensions, but it can be overcome by accelerating the formation of the DA reaction network. In this presentation, formation of DA networks was observed rheologically over the course of the curing process. Furan- and maleimide-functionalized precursors of varying architecture, functionality, and molecular weight were synthesized. DA networks cured from the precursors were tested for their thermomechanical properties through calorimetry and rheometry. DA networks formed of flexible networks were shown to behave more elastomeric compared to those of rigid networks. The samples showed a moduli drop and an endothermic reaction at ~120°C indicative of the depolymerization of the DA network. The gelation time, which represents network formation across the reaction system, decreased with increasing rigidity of the network. These results can be used to develop reversible thermosets that can be printed and used without a post-curing step.
**Structural and Mechanical Properties of Compositionally Complex Alloys from First-Principles DFT**

Susan R. Atlas\textsuperscript{1,2}, Surya Bijjala\textsuperscript{3}, Pankaj Kumar\textsuperscript{3}

\textsuperscript{1} Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131
\textsuperscript{2} Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131
\textsuperscript{3} Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131

**Speaker Name – Susan R. Atlas**

**INVITED PRESENTATION**

**Abstract** –

The rational design of materials for extreme temperature applications, including the use of empirical machine learning approaches, is an active area of contemporary research. Recent attempts have revolved around alloys of the refractory bcc metals Mo, W, Nb, and Ta, due to their high melting temperatures. Target materials criteria include manufacturability and the optimization of mechanical properties such as high-temperature strength, room-temperature ductility, and fracture toughness. In order to accurately balance competing quantum mechanical energetic and entropic effects contributing to optimal alloy design, we have performed density functional supercell studies of the elemental materials and their binary disordered bcc alloys (NbMo, NbTa, NbW, MoTa, MoW, and TaW). Building on these results, we present a systematic approach to the direct, multiscale prediction of ductility and yield strength in alloys of increasing complexity, as a function of composition.
A First-Principles Study of Calculation Parameters Affecting Diffusion and Creep Activation Energy in the CoCrNi Medium-Entropy Alloy

Chelsea Hargather¹, Christopher Lafferty¹

¹ New Mexico Institute of Mining and Technology

Speaker Name – Chelsea Hargather

Abstract –

High-entropy alloys (HEAs) are potential candidates for high-performance engineering material applications. Creep is permanent, time-dependent inelastic deformation under applied stress, and diffusion properties are an important contribution to secondary creep behavior. In the present work, first-principles calculations are employed to analyze activation energy for diffusion in the CoCrNi system. The effects of various calculation parameters, including the magnetic and non-magnetic states, and two versions of the generalized gradient approximation, are compared. Widom-type substitution techniques are used. Special quasi-random structures (SQS) are employed, and complications related to the structural complexity and magnetism when using first-principles techniques are discussed. The relationship between the creep-activation energy and diffusion-activation energy in well studied systems, such as CoCrNi, is explored. Results are compared to known literature where available, and the importance of the calculations for novel alloy design are discussed.
Unsupervised Physics-Informed Disentanglement of Multimodal Materials

Data
Carianne Martinez\textsuperscript{1,2}
\textsuperscript{1} Applied Machine Intelligence, Sandia National Laboratories, Albuquerque, NM
\textsuperscript{2} Arizona State University

Speaker Name – Carianne (Cari) Martinez
**INVITED PRESENTATION**

Abstract –

Materials are commonly evaluated via a variety of experimental modalities, each individually describing some aspect of the process conditions, material structure, chemistry, material properties, and associated performance. We seek to identify fingerprints within this multimodal data - signals associated with desirable material properties - that may be used to accelerate discovery of resilient materials. We introduce physics-informed multimodal autoencoders (PIMA) - a variational inference framework for discovering shared information in multimodal scientific datasets representative of high-throughput testing. Individual modalities are embedded into a shared latent space and fused through a product of experts formulation, enabling a Gaussian mixture prior to identify shared features. Sampling from clusters allows cross-modal generative modeling, with a mixture of expert decoder imposing inductive biases encoding prior scientific knowledge and imparting structured disentanglement of the latent space. This approach enables discovery of high-dimensional fingerprints that allow the correlation of complex fused material descriptors to corresponding material properties and uncertainty quantification to determine the relative information value of each source modality.
Effect of In-Liquid Phase Separation on Non-Classical Nucleation in Al-Fe Alloys: A Molecular Dynamics Study
Md Mahmudul Hasan¹, Deep Choudhuri¹

¹ New Mexico Institute of Mining and Technology, Socorro, NM, 87801

Abstract –

Emergence of in-liquid metastable structures during alloy solidification can result in multi-step nucleation process, which is often referred to as non-classical nucleation. From a mechanistic standpoint, such metastable structures have a strong tendency to transform into a thermodynamically equilibrium structure. For example, Aluminum-based alloys are expected to form the equilibrium face-centered-cubic (FCC) phase upon solidification. However, several studies have shown that metastable hexagonal-close-packed (HCP) forms first, and, subsequently, transforms to stable FCC within the undercooled liquid. Interestingly, these studies rarely interrogated the effect of solute segregations on non-classical nucleation. We have probed this matter in Al-Fe alloys, by performing classical molecular dynamics simulations that employed modified embedded atom method (MEAM) potential. Our results indicated liquid Al-Fe alloy phase separates into two distinct Fe-rich and Al-rich domains. Nucleation is initiated within the Al-rich domain by forming HCP clusters. These clusters later transformed into FCC consistent with extant literature. However, the extent of HCP-to-FCC transformation depended on the size of Fe-rich domains. We found that higher Fe concentration yielded larger domains and hindered the FCC nucleation. Our results demonstrate that non-classical nucleation is also affected by local solute segregations within an undercooled liquid.
Effect of Thermal Gradient on Interfacial Free Energy and Anisotropy

Parameters in Al-Cu Alloy

Amrutdyuti Swamy¹, Pabitra Choudhury¹, Anthony Lavelle¹

¹Department of Chemical Engineering, New Mexico Tech, Socorro, NM, 87801

Speaker Name – Amrutdyuti Swamy

Abstract –

Additive manufacturing (AM) has established itself as a transformative approach in manufacturing, offering advantages such as the capability to produce intricate geometries, minimized waste, and the creation of tailored parts. However, a limited range of metals and alloys are suitable for AM due to the onset of microscopic defects such as cracks and porosity during solidification. Additive manufacturing of Al-Cu alloys also remains a challenge due to these reasons. A suggested strategy focuses on increasing the proportion of equiaxed grains relative to the elongated columnar grains in the microstructure to reduce these micro-defects. This study delves into methods to enhance the proportion of equiaxed grains in Al-Cu alloys during the rapid solidification process. Utilizing molecular dynamics simulations, we examine the solid-melt interface of an Al-Cu system by varying the Cu composition and the thermal gradient. Previous investigations indicated that elevating the Cu content beyond 8.8 at. % can promote the formation of more 110 oriented equiaxed grains over the 100 oriented columnar grains. Current work extends this by introducing a thermal gradient across the solid-melt boundary to simulate in-situ rapid solidification conditions. We assess the combined effect of Cu composition and thermal gradient on the final microstructure. Furthermore, we also compute the evolution of interfacial free energy and anisotropy parameters in relation to the applied thermal gradient.

PC would like to acknowledge the support from U.S. Army Research Laboratory and New Mexico Institute of Mining and Technology cooperative agreement No. W911NF2020190. Acknowledgment is also made to the State Legislative Fund, New Mexico for financial support. This work used Stampede 2 at TACC through allocation [TGDMR140131] from the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) program, which is supported by National Science Foundation grants #2138259, #2138286, #2138307, #2137603, and #2138296. This work also 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.
Microstructural Black Swans
Brad Boyce¹

¹Sandia National Laboratories, Center for Integrated Nanotechnologies, Albuquerque, NM

Speaker Name – Brad Boyce
**INVITED PRESENTATION**

Abstract –

Black swans are a metaphor for rare events with extreme consequences. In the domain of structural materials, black swans represent features in the microstructure that lead to catastrophic failure; as a result of their rarity, they are difficult to observe and often overlooked. These unusual weakest-link features are described variously as incipient, emergent, or anomalous. They give rise to localization, percolation, or avalanche events such as fracture, ductile rupture, dielectric breakdown, corrosion pit nucleation, and fatigue-crack initiation; as such, they are limiting cases in the concept of a representative volume. In this perspective, three examples are given of rare microstructural features and how they limit the mechanical reliability of structural metals. After taking stock of these examples, a future outlook considers the need for high-throughput testing and non-destructive characterization as well as detection algorithms and materials modelling strategies, including accelerated machine learning methods, that can capture anomalous events.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
**Fully Removable Epoxy Utilizing Dynamic Covalent Bonds with Comparable Adhesive Strength to Conventional Epoxy**

Samantha (Lindholm) Knight\(^1\), Gaeun Kim\(^1\), Nicole Penners\(^1\), Sanchari Chowdhury\(^1\), John McCoy\(^2\), Youngmin Lee\(^1\)

\(^1\) Department of Chemical Engineering, New Mexico Tech, Socorro, NM, 87801
\(^2\) Department of Materials Engineering, New Mexico Tech, Socorro, NM, 87801

Speaker Name - Samantha (Lindholm) Knight

**Abstract** -

Conventional epoxies have a variety of features that make them appealing for adhesive purposes. Their stability under different conditions makes them an ideal choice for adhesion to almost any substrate. However, their thermosetting nature makes them permanent and nearly impossible to remove without damaging the adhered surfaces. Introduction of Diels-Alder (DA) dynamic bonds into the epoxy network is one method to overcome this limitation. DA chemistry has both a forward and a reverse reaction. The two competing reactions have an equilibrium that is temperature dependent. The forward reaction occurs at lower temperatures, making the material a glassy solid. Above \(\sim 120^\circ C\) the reverse reaction is dominant, which breaks the dynamic bonds and depolymerizes the network. At the higher temperatures the depolymerized epoxy can flow, and upon cooling it re-solidifies. This property of the DA epoxy overcomes the major limitation of conventional epoxy adhesives. In this study, adhesive strength of DA epoxies have been studied at various temperatures to see their potential application for removable adhesives. DA epoxies with various architectures of a network are used to adhere substrates. They are then pulled while measuring the stress necessary to separate the substrates. Because of the thermal dependence of the DA reverse reaction, the adhesive strength varies greatly with temperature. Plasmonic nanoparticles can also be incorporated to have a photothermal effect, controlling the adhesive strength with light. The adhesive strength of the DA epoxy can then be compared to conventional formulations.
Strain-Path Dependent Dislocation Evolution in Aluminum 6016

Sarah Sanderson¹, Rishabh Sharma¹, Asher Webb¹, Michael Miles¹, Marko Knezevic², David Fullwood¹

¹ Brigham Young University
² University of New Hampshire

Speaker Name – Sarah Sanderson

Abstract -

In recent efforts to reduce carbon emissions and improve fuel economy, car manufacturers have pursued replacing conventional steel in automotive structures with lightweight alloys. High strength aluminum alloys, such as the Al 6xxx series, are compelling candidates; however, the limited room-temperature formability of the alloys, along with difficulty in predicting final shape due to springback hinders their widespread application. A better understanding of deformation at the microstructural level, specifically relating to statistically stored (SSD) and geometrically necessary dislocation (GND) evolution and related internal stress development, will provide information critical to the development of reliable forming techniques for high strength aluminum. After subjecting Al 6016-T6 to strain-path & changes in uniaxial and plane strain tension, we employ high-resolution electron backscatter diffraction (HREBSD) cross-correlation techniques and x-ray diffraction (XRD) analysis to map GND subgrain structure development and overall dislocation density, respectively. An additional two-point statistical analysis on GND data reveals clustering of GNDs around precipitates rather than grain boundaries challenging the well-established idea that grain boundaries are perhaps the primary barriers to dislocation slip in Al 6016 deformation.
**Abstract -**

It is a frequent challenge in crystal plasticity to determine when an experiment and a computational model disagree, is it due to limitations of the model, or is there a stochasticity to the material’s response where different responses are both possible? In experimental crystal plasticity, experimentalists are often limited to choosing what test they can complete on a single specimen as many tests are both destructive in nature and not combinable leaving scientists to interpret how different tests on non-identical microstructures can be related to each other. Microstructural clones introduce a solution to each of those issues. Microstructural clones are oligocrystal specimens that have nearly identical microstructures. Having specimens with nearly identical microstructures allows for ‘repeat’ destructive tests of a microstructure that provides an understanding of stochasticity within a microstructure as well as an ability to ‘see the future’ to understand where and when a specimen will deform. This capability allows for future small scale measurements knowing locations of stress concentrations and interesting behaviors without depending on notching or other forms of manipulating a specimen’s geometry. Experimental crystal plasticity using pure nickel microstructural clones are being used in this study to improve computational crystal plasticity models.

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Accelerating Materials Simulations with Machine-Learning Strategies

Remi Dingreville\textsuperscript{1}

\textsuperscript{1}Center for Integrated Nanotechnologies, Sandia National Laboratories

Speaker Name – Remi Dingreville

**INVITED PRESENTATION**

Abstract -

Mesoscale direct numerical simulations (DNS) such as phase field or crystal plasticity are accurate but computationally expensive, requiring high-performance computing resources and sophisticated numerical integration schemes to achieve a useful degree of accuracy. In this talk, I will discuss how we can go beyond these limitations by merging computational materials science and machine-learning tools. I will discuss two strategies. The first strategy is based on a fast and generalizable surrogate model that integrates a low-dimensional representation of the material with a history-dependent neural network. In this case, the machine-learning solver replaces the DNS solver. I will illustrate this strategy on phase-field simulations for the time evolution of microstructure in binary alloys. The second strategy is based on a physics-informed, multi-layer neural network which uses physical governing equations as its building blocks. Here the neural network acts as a reduced-order model replacing DNS. I will illustrate this strategy on the thermo-mechanical response of composite materials. For both of these strategies, I will discuss how the type of speed one can gain and how we can harness these emerging techniques for materials design and process optimization.

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Thermodynamic properties as a function of temperature of AlMoNbV, NbTaTiV, NbTaTiZr, AlNbTaTiV, HfNbTaTiZr, and MoNbTaVW refractory high-entropy alloys from first-principles calculations

Danielson Moreno¹, Chelsey Hargather¹

¹ New Mexico Institute of Mining and Technology

Speaker Name - Danielson Moreno

Abstract -

Refractory high-entropy alloys (RHEAs) are strong candidates for use in high-temperature engineering applications. As such, their thermodynamic properties as a function of temperature for a variety of systems need to be studied. In the present work, properties such as entropy, enthalpy, heat capacity at constant volume, and linear thermal expansion are calculated for 3 quaternary and 3 quinary single-phase, BCC RHEAs. First-principles calculations based on density functional theory are used for the calculations, and special quasirandom structures are used to represent the random solid solution nature of the RHEAs. A code for the finite temperature thermodynamic properties using the Debye-Einstein model is written and employed.
Leveraging Kinetic Monte Carlo to Characterize Early Stages of Nonclassical, Molecular Crystallization in Resveratrol

Tesia Janicki¹, Christine Roberts¹, Helen Cleaves¹, Christopher Brotherton¹, Rekha Rao¹, Theron Rodgers¹

¹ Sandia National Laboratories, Albuquerque, NM

Speaker Name – Tesia Janicki

Abstract -

Resveratrol (3,5,4-trihydroxy-trans-stilbene) exhibits antioxidant and antimicrobial properties and has been proposed for use in both anticancer and antiaging therapies. Such organic compounds are typically purified via recrystallization in solution. While classical crystallization proceeds through a nucleation-and-growth mechanism, nonclassical crystallization is preceded in growth by a multistep nucleation process involving intermediate phases or aggregation of primary particles. To characterize nonclassical crystallization in resveratrol, we pursue a multi-scale approach spanning experiment and theoretical methods. This work focuses on atomistic simulation of crystallization via kinetic Monte Carlo (kMC). First, we introduce the structure of resveratrol and discuss approximations used in an on-lattice kMC model. Second, we summarize modifications to the Stochastic Parallel PARticle Kinetic Simulator (SPPARKS) package to run our kMC model. Finally, we discuss benchmarking crystal deposition events using DFT and preliminary results for crystal growth. Ongoing work connects kMC predictions to experimental observation to define a mechanism for nonclassical crystallization.

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First-Principles-Based Computation of Ground State Properties of Heavy

Refractory Elements and Binaries

Surya Bijjala\textsuperscript{1,2,3}, Susan R. Atlas\textsuperscript{2,3}, Pankaj Kumar\textsuperscript{1}

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\textsuperscript{1}Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131
\textsuperscript{1}Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131

Abstract -

High entropy alloys offer a vast unexplored compositional space that requires ability for high throughput screening of the compositions for targeted properties. First-principles density functional theory (DFT) methods enable the quantum mechanical determination of ground state materials properties from atomic constituents, with only a few input parameters. However, the accuracy of DFT-predicted materials properties can significantly depend on the selection of DFT methodology and computational parameters. For accurate prediction of materials properties, the chosen computational parameters need to be consistent across the constituent elements. Here, we present benchmarking studies for systematic determination of computational parameters for elemental and binary alloys refractory alloys of Mo, W, Nb and Ta. We report calculations of the lattice constant (\(a\)), bulk modulus (\(K\)), cohesive energy (\(E\)), elastic constants, and surface energies of (100), (110), (111) for elemental Mo, W, Nb, and Ta, using the Abinit DFT electronic structure code \cite{Abinit}, and compare results using the FHI (considers only d valence electrons) and pseudo-dojo (considers s, p and d valence electrons) norm-conserving pseudopotentials (NCPP), and projector augmented-wave (PAW) (considers s, p and d valence electrons) pseudopotentials. We also report lattice constants (\(a\)), bulk modulus (\(K\)), cohesive energy (\(E\)), elastic constants, for binary NbMo, NbTa, NbW, MoTa, MoW, TaW. Computed properties using pseudo-dojo NCPP and PAW pseudopotentials agree well with other theoretical calculations and with experiments.
A Hybrid Aerosol Jet Printing and Electrodeposition Process for the Manufacturing of Multi-Layer Flyback Transformers

Lok-Kun Tsui\textsuperscript{1,2}, Thomas Hartmann\textsuperscript{2}, Joshua Dye\textsuperscript{2}, Judith Lavin\textsuperscript{2}

\textsuperscript{1} University of New Mexico, Center for Micro-Engineered Materials, Albuquerque, NM
\textsuperscript{2} Sandia National Laboratories, Albuquerque, NM

Speaker Name - Lok-Kun Tsui

Abstract -

Flyback transformers made from additively manufactured planar inductors are a promising technology for lightweight, robust power electronics applications. Aerosol jet printing (AJP) is a direct write additive manufacturing technique that can achieve 10 µm resolution while supporting a wide range of metals, insulating dielectrics, and other materials of interest to printed electronics. However, the AJP of metals is limited by the low conductivity of nanoparticle inks and the inaccessibility of materials such as Cu. In this work, we demonstrated a combined AJP and electrochemical deposition process for manufacturing of flyback transformers consisting of a 3-turn per layer 2-layer primary inductor and a 31-turn per layer 2-layer secondary inductor. AJP of Ag served as seed layers, which was followed by electroless and electrodeposition of Cu and Ni. This hybrid process allows us to access both the high conductivity and density of electrodeposited material while maintaining the high-resolution patterning of AJP. The UV-curable dielectric polymer Norland Optics NOA61 was also printed by AJP as separation layers. Inductances of 199-206 nH and 19-23 µH for the primary and secondary inductors respectively were measured by impedance and agreed with COMSOL simulations in both 2D axisymmetric and 3D models. Operating in a coreless configuration, the flyback transformer converted an input voltage of 17 V at 400 kHz to 1250 V, a gain of 73.5x. When integrated with Fe4N magnetic layers, the gain increased to 100x.

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**Process Optimization for Wire Arc Additive Manufacturing**

Natalia Saiz\(^1\), Hannah Sims\(^1\), Shaun Whetten\(^1\), Levi Van Bastian\(^1\), Jonathan Pegues\(^1\)

\(^1\)Sandia National Laboratories, Albuquerque, NM

Speaker Name – Natalia Saiz

Abstract -

Directed energy deposition (DED) is an additive manufacturing (AM) process that builds components layer by layer and is useful for larger components. DED has been identified as a potential solution for net shape manufacturing of metals with increased the build rate and build volume when compared to conventional additive manufacturing processes. Despite these benefits, several process challenges remain such as non-ideal microstructures and system monitoring. DED processes generally require physical surveillance for the duration of the process, which can be problematic for increasingly large parts with long run times typically over ten hours. Within this work, we focus on a wire arc additive manufacturing (WAAM) utilizing tungsten inert gas (TIG) deposition process. Optimization of the process-structure-property relationships was explored, targeting an increase in the deposition rate of this procedure while simultaneously improving the structure-property couplings. Results are discussed in the context of total build time for a development build correlating process changes to the resulting grain morphology and mechanical properties.

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Physical Properties of ARB Cu/Nb Nanolamellar Composites

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¹ Department of Nuclear Engineering, University of New Mexico, Albuquerque, NM

Speaker Name – Jared Justice

Abstract –

Nanolamellar composites with high interface density have increased strength due to interfaces serving as barriers to dislocation movement and high radiation damage resistance due to these interfaces serving as point defect sinks. However, these interfaces also serve as barriers to electron and phonon motion, reducing the electrical resistivity and thermal conductivity. This work seeks to understand the inherent tradeoff between strength and physical properties of nanolamellar composites produced by accumulative roll bonding. Specimens with layer thickness ranging from 25 nm to 193 nm were studied. The electrical resistivity was investigated over temperatures ranging from 0 K to 300 K. The effect of longitudinal rolling and cross rolling was also investigated. Electrical resistivity results were then compared with two models for resistivity of thin-films: the Fuchs-Sondheimer and the Mayadas-Shatzkes models. The thermal conductivity of the specimens was evaluated using modulated thermoreflectance. Findings showed that while resistivity increased with decreasing layer height, thermal conductivity was only weakly dependent on layer height. The material showed significant anisotropy in both in-plane directions and cross-plane directions.
**Fatigue Behavior of Additively Manufactured Ti-5553**

Zachary Casias\(^1\), Jay Carroll\(^1\), Pankaj Kumar\(^2\), Christopher Laursen\(^1\)

\(^1\) Sandia National Laboratories, Albuquerque, NM  
\(^2\) University of New Mexico, Albuquerque, NM

Speaker Name – Zachary Casias

**Abstract** -

One of the most common high-strength alloys used in additive manufacturing is Ti-6Al-4V. However, due to its poor thermal conductivity, high strength, and relatively low ductility, large components made of Ti-6Al-4V tend to experience cracking due to residual stresses. The near-beta titanium alloy, Ti-5Al-5Mo-5V-3Cr (Ti-5553), provides a potential solution with a lower as-printed yield strength that can be later heat treated to higher strength. To date, the mechanical properties of Ti-5553 are not documented sufficiently in the published literature. Even less information exists for additively manufactured (AM) Ti-5553. This work studies the fatigue behavior of AM Ti-5553 with particular focus on heat treatment effects. Comparisons are made with studies in AM Ti-6Al-4V and conventionally manufactured Ti-5553. The role of flaws plays an important role in fatigue and strategies for quantifying their effects is also addressed.

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Coke-Resistant Single Atom Catalyst for Hydrogen Production via Methane Pyrolysis

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¹ Department of Chemical Engineering, New Mexico Tech, Socorro NM 87801
² Department of Chemistry, New Mexico Tech, Socorro NM 87801

Abstract -

The growing emphasis on sustainable hydrogen production from natural gas, coupled with carbon capture, has revitalized the study of methane pyrolysis. Methane pyrolysis includes successive C-H bond activations from methane to produce hydrogen gas and solid carbon. Existing catalysts are prone to deactivation due to the buildup of coke on their surfaces. This coke formation is linked to the strong attachment of CH₂ intermediate fragments and exothermic reaction pathway. To be effective, a catalyst needs to be able to activate C-H bond effectively while resisting coke formation. Recently, single Ni atoms have been reported to be deposited on titanium nitride (TiN) plasmonic nanoparticles and that the single Ni atoms favorably deposit on N-vacancy sites on the TiN surface. Supported by computational results, single atom catalyst (SAC) formation has been confirmed through experimental TEM imaging and XPS results. Utilizing ab initio spin-polarized DFT calculations, this study investigates the behavior of transition states for methane pyrolysis and the associated activation energy barriers on SAC Ni sites supported by titanium nitride (Ni-TiN). The highest activation energy barrier was found to require 1.10 eV. Additionally, the weaker bonding to adsorbates and an overall endothermic reaction pathway suggests that Ni-TiN is likely to prevent the accumulation of coke on its surface, allowing it to remain active.

Acknowledgment is made to the State Legislative Fund, New Mexico for financial support. This work used Stampede2 at TACC through allocation [TGDMR140131] from the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) program, which is supported by National Science Foundation grants #2138259, #2138286, #2138307, #2137603, and #2138296. This work also 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.
Mixed Potential Electrochemical Sensors for Methane Emissions Monitoring

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¹ University of New Mexico, Albuquerque, NM
² SensorComm Technologies, Albuquerque, NM
³ Sandia National Laboratories, Albuquerque, NM

Speaker Name – Sleight Halley

Abstract -

Sensors for continuous monitoring of methane emissions from natural gas infrastructure are needed to mitigate the impact of this potent greenhouse gas on global climate. Solid-state mixed potential sensors are a robust, low-cost sensing technology suitable for field deployment. We have developed ceramic additive manufacturing technologies for prototyping of sensors consisting of magnesia-stabilized zirconia substrates, metal and metal oxide electrodes, and yttria-stabilized zirconia porous electrolytes. The substrate material was selected to have low ionic conductivity to promote optimal isolation of the electrodes which resulted in a demonstrated limit of detection below 40 ppm of CH₄ in simulated natural gas mixtures. The sensors were then integrated into a portable platform capable of collecting sensor data and transmitting the results to a cloud server. Field testing was performed at Colorado State University’s Methane Emissions Technology Evaluation Center and successfully quantified methane originating from a buried pipeline. This work was supported by US DoE Award DEFE0031864.
Freeform Liquid Crystal Elastomers via Embedded 4D Printing

Luke McDougall 1, Jeremey Herman1,2, Emily Huntley 1, Adam Cook1, Timothy White 2, Bryan Kaehr 1, Devin J. Roach1,3*

1 Advanced Materials Laboratory, Sandia National Laboratories, NM, USA
2 Chemical Engineering Department, The University of Colorado, Boulder, CO
3 Department of Mechanical, Industrial, and Manufacturing Engineering, Oregon State University, Corvallis, OR

Speaker Name - Luke McDougall

Abstract -

Liquid crystal elastomers (LCE) are a class of active material that can generate rapid, reversible mechanical actuations in response to a variety of stimulus. Fabrication methods for LCE have remained a topic of intensive research interest in recent years. Photopatterning and two-stage reaction techniques were pioneering methods which enabled molecular patterning and fabrication of LCE networks in few, relatively simple steps. Recently, additive manufacturing (AM), or 3D printing, has become another promising approach for facile production of LCE networks. The combination of 3D printing with responsive materials, such as LCE, has led to a new generation of smart structures that not only possess a static shape but also can change their shape over time. This process is termed 4D printing, with the fourth dimension being time. To date, 4D printed LCE structures have been limited to flat objects and therefore possess inadequate shape complexity and associated actuations for most smart structure applications. In this work, we report the use of embedded 4D printing to extrude LCE ink into a gel media to produce freestanding, geometrically complex 3D architectures. Due to the hydrophobic nature of the LCE ink, a 96wt% water gel was developed, allowing for high-resolution printing without sacrificing LCE alignment and mechanical actuation properties. This approach enables LCE molecular programming in any 3D cardinal direction generating unique 3D to 3D shape transformations. The ability to 4D print complex, freestanding 3D LCE architectures opens new avenues for the design and development of functional and responsive systems such as reconfigurable metamaterials, soft robotics, or biomedical devices.
**In-situ Process Monitoring of Direct-Ink Write Printing**

Jessica Kopatz\(^1\), Derek Reinholtz\(^1\), Jonathan Leonard\(^1\), Alexander S. Tappan\(^1\), Adam W. Cook\(^1\),
Anne M. Grillet\(^1\)

\(^1\) Sandia National Laboratories, Albuquerque, NM

Speaker Name – Jessica Kopatz

**Abstract -**

Additive manufacturing enables the creation of unique, custom-designed hardware in a relatively timely and inexpensive manner. Adoption of the technology could be enhanced by increasing confidence in the quality of the final part by using process monitoring. Direct-ink write (DIW) operates by extruding a particle-filled ink onto a substrate in a desired pattern via extrusion through a syringe. Defects in the printed part can be caused by trapped air or particle aggregates within the ink, some of which can be as extreme as clogging of the syringe nozzle during extrusion. These defects can be detrimental to the quality of the printed part through problems with shape tolerance due to under or over extrusion or changes to final material properties. Modifying the extrusion apparatus through the addition of pressure sensors, located at the top and bottom of the syringe, can aid in identifying detection of potential defects during printing. The sensitivity of the pressure monitoring is investigated using engineered spherical defects in a range of sizes from 106-1000 micron mixed into DowSil SE1700. Pressure measurements could detect particle aggregates larger than 60% of the nozzle diameter, thus providing helpful information for understanding DIW print quality.

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Characterization of Viscous and Performance Properties of APCP for Application to Additive Manufacture

Dylan Purcell¹, Michael Hargather¹, Chelsey Hargather²

¹ Department of Mechanical Engineering, New Mexico Institute of Mining and Technology
² Department of Materials Engineering, New Mexico Institute of Mining and Technology

Speaker Name – Dylan Purcell

Abstract -

Solid rocket propellant has many applications for additive manufacture, but the process is complex. Understanding of the viscous properties of the uncured propellant during additive is critical for proper deposition. These properties are heavily influenced by the total amount of solids suspended within the polymeric binder, as well as the distribution of the sizes of the particles themselves. The viscous behavior of seven formulations of ammonium perchlorate composite propellant (APCP), along with 7 non-curing variants, were tested in this study. The most promising materials for additive manufacture exhibited apparent viscosities between 4 and 8 million cP, with non-Newtonian behavior similar to a Bingham plastic. The formulations were then cured and formed into burn strands to determine the burn rate of the materials. Burn rates ranged between 1.2 and 1.7 mm/s, which, while on the lower end of propellant burn rates, is considered acceptable due to the composition. The results of the test demonstrate materials that are viable for different forms of additive manufacture and show promising performance characteristics for use as a propellant.
Combustion Rates as a Function of Thermite Content for an Energetic Initiator Ink

Kayleigh Cameron¹, Chelsey Hargather¹

¹ Department of Materials Engineering, New Mexico Institute of Mining and Technology

Speaker Name – Kayleigh Cameron

Abstract -

Additive manufacturing has the ability to expand the applications of energetic materials by eliminating several problems faced in traditional manufacturing. The goal of this project is to create an energetic initiator ink made from a polymer binder, a metal fuel, and a metal oxide for additive manufacturing that can be produced to ignite less sensitive materials, have a wide range of geometries, and have tailorable burn properties. An important aspect in creating a printable material with these tailorable burn properties is the characterization of burn rate and density as a function of composition variables. This work focuses on the analysis of burn rate and density as a function of the percentage of iron sulfur (Fe-S), which undergoes a high heat producing redox reaction but is more controllable compared to pure thermite, and the percent solids loading in strontium nitrate (Sr(NO₃)₂), barium nitrate (Ba(NO₃)₂), and manganese oxide (MnO₂) and aluminum thermite systems. It has been found that increasing the percentage of Fe-S decreases the burn rate, with the maximum burn rate for each composition being at either 15% or 25% Fe-S. It was also found that increasing the percentage of Fe-S increases the density of each system.
Experimental Assessment of Additively Manufactured Copper Solderability

Joseph Erwin\textsuperscript{1,2}, Benjamin C. White\textsuperscript{1}

\textsuperscript{1} Sandia National Laboratories, Albuquerque, NM
\textsuperscript{2} University of New Mexico, Albuquerque, NM

Speaker Name – Joseph Erwin

Abstract –

Additive manufacturing (AM) of metals is a wave of the future with immense potential and proven ability to benefit industry. Relatively recent advancements in AM technology have allowed for production of copper by Laser Powder Bed Fusion, Laser Engineered Net Shaping, and Bound Powder Extrusion. Copper’s high electrical conductivity could make AM production with this element hugely beneficial to circuit component production. Of course, these AM copper components must make electrical connections to the circuit, likely with solder. To understand the solderability of AM copper, coupons produced by the afore mentioned methods had their solderability experimentally characterized by the wetting balance technique and pin pull testing. The coupons were tested as built and after surface modification by dry electropolishing. It was found that dry electropolishing improved the solderability of copper produced by all three methods and that bound powder extrusion produces the best surface for solderability.

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3D Printing of Conversion Cathodes for Enhanced Custom-Form Lithium Batteries

Jorge Cardenas¹,²,³, John Paul Bullivant¹, Bryan Wygant¹, Laura Merrill¹, Aliya Lapp¹,², Timothy Lambert¹, Eric Allcorn¹, A. Alec Talin², Adam W. Cook¹, Katharine L. Harrison¹,³

¹ Sandia National Laboratories, Albuquerque, NM
¹ Sandia National Laboratories, Livermore, CA
¹ National Renewable Energy Laboratory, Golden, CO

Speaker Name – Jorge Cardenas

Abstract

Additive manufacturing techniques can enable the fabrication of batteries in nonconventional form factors, enabling higher practical energy densities due to improved power source packing efficiency. Furthermore, energy density can be improved by transitioning from conventional Li-ion materials to lithium metal anodes and conversion cathodes. Iron disulfide (FeS₂) and iron trifluoride (FeF₃) are two promising conversion cathodes of commercial and academic interest, but the 3D printing of inks made from these materials for custom-form battery applications has yet to be demonstrated. In this work, the deposition of FeS₂ and FeF₃ inks are investigated and optimized using direct-ink-write (DIW) 3D printing, in addition to the development of printable separators and packages to produce custom-form batteries. Two distinct custom form-factors, one on wave-shaped current collectors and the other on cylindrical rod current collectors, are demonstrated and shown to exhibit performance similar to coin cells when conventional Celgard separators are used. Additionally, FeF₃ cells were integrated with a DIW printed separator consisting of an electrolyte exchanged PVDF-HFP based ionogel [1]. In the case of FeS₂, it was found that cathodes with a ridged surface, produced from the filamentary extrusion of highly concentrated inks (60-70% solids w/w%) exhibited optimal power, uniformity, and stability [2]. Finally, progress toward fully-printing custom-form batteries using metal powder bed printed cases and printed polymer gaskets is demonstrated. Overall, the additive manufacturing of conversion electrodes, separators, and battery packaging is shown to be a viable path toward the making of custom-form cells. More broadly, electrode ridging is found to optimize rate capability, a finding that may have broad impact beyond FeS₂, FeF₃ and additive manufacturing.

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