Rio Grande Symposium 2026 Abstracts

Oral Presentations

Tungsten-Integrated Photopolymer Composites for Extreme Chemical and Radiation Environments Fabricated via Vat Photopolymerization

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Advanced nuclear, space, and radiochemical processing technologies require structural materials that can withstand both ionizing radiation and aggressive chemical environments, a combination no commercially available 3D-printable material currently meets. This gap is especially critical for nuclear facilities needing custom-geometry flow devices, containment fixtures, and shielding components with high dimensional precision. To address this, we developed a photopolymer resin for vat photopolymerization based on a hydrophobic aromatic acrylate system loaded with a tungsten-based filler. Printed parts were aged in aggressive acids, bases, and solvents to evaluate chemical inertness, showing strong mechanical and thermal performance with sustained structural integrity throughout extended exposure. The optimal AMT loading outperformed both lower-loaded formulations and commercial photopolymer resins in chemical durability, retaining most of its tensile strength and modulus even after prolonged solvent exposure. Silane treatment of the filler further improved chemical resistance and print resolution through enhanced particle dispersion. Gamma radiation compatibility testing is ongoing. This work establishes a manufacturable platform for chemically durable, tungsten-loaded composites, laying the foundation for materials capable of withstanding both radiation and chemical extremes.

Identifying a Novel Gate-Drain Leakage Mechanism in GAAFET Using Quantum Transport Simulations

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GAAFETs are emerging as the leading architecture for continued transistor scaling beyond FinFET technology. Although the gate-all-around geometry provides improved electrostatic control and reduced short-channel effects, experimental measurements reveal an unexpected increase in drain current as the gate voltage becomes more negative. Understanding the origin of this leakage is important for determining the scaling limits of GAAFETs and reducing off-state power consumption.

In this work, we use quantum-transport simulations based on the Non-Equilibrium Green Function (NEGF) and the Contact Block Reduction (CBR) method to identify the physical origin of this leakage by evaluating the current at the terminals and the different potential current paths. Firstly, our quantum-transport simulations reproduce the measured I-Vg characteristics for positive and negative gate voltages. At positive gate voltages, our simulations indicate that the drain current is dominated by source-drain current, while the gate-current components remain several orders of magnitude smaller. At negative gate voltages, however, the gate-drain current increases and becomes the dominant component of the total drain current. Further analysis demonstrates that the applied drain bias lowers the effective dielectric tunnel barrier between the gate and drain while leaving the gate-source barrier relatively unchanged. This drain-induced dielectric barrier lowering exponentially enhances direct electron tunneling through the high-k dielectric and explains the strong drain-bias dependence of the measured leakage.

These results demonstrate the importance of treating the gate as a quantum-mechanical contact when modeling ultra-scaled transistors. The simulations also suggest mitigation strategies, including locally increasing the dielectric thickness or using a higher-barrier dielectric near the drain side of the gate.

Effect of Rhenium Content and Annealing Temperature on Microstructure and Mechanical Properties of Molybdenum-Rhenium Alloys

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This study investigates the influence of rhenium concentration and annealing temperature on the microstructure and mechanical properties of molybdenum-rhenium (MoRe) alloys. MoRe alloys with rhenium contents ranging from 5 to 41 wt.% are examined in the as-received condition and after annealing treatments ranging from 800°C to 1450°C. The microstructural evolution is characterized using scanning electron microscopy and electron backscatter diffraction to evaluate grain size, texture, and recrystallization behavior. Mechanical properties are assessed through bulk compression testing, Vickers hardness, and nanoindentation to compare macroscopic and localized deformation responses. By correlating composition, heat treatment, and mechanical performance, this work aims to understand how rhenium content influences grain growth, recrystallization temperature, and strength in MoRe alloys. These results provide insight into processing-structure-property relationships that can guide optimization of refractory alloys for high-temperature applications and extreme environments.

Strong Radial Electric Field Scaling Near Nanoscale Conductive Filaments and the ReRAM Reset Mechanism

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Filamentary analog Resistive Random Access Memory (ReRAM) has long been considered a leading candidate for embedded digital memory and weight representation in neuromorphic computing accelerators. The negative (reset) resistance switching mechanism in filamentary devices remains contentious. The lack of understanding of the reset mechanism has been identified by reviews on the subject as the primary barrier to ReRAM technology development. This study introduces a nanoscale effect in current carrying conductors, whereby surface charge induced radial electric fields are found to be inversely proportional to the radius of the conductive path. This novel nanoscale effect is then successfully applied to explain the negative resistance switching (reset) mechanism in bipolar filamentary resistive switching memory devices (memristors). The physics underlaying reset in bipolar resistive memory has been the subject of decades of controversy and has been identified as the primary barrier to resistive memory technology development. Previous explanations for the negative resistive switching mechanism state that diffusion constitutes the radial driving mechanism for mobile ions with drift under electric fields is restricted to the direction parallel current flow. This explanation conflicts with retention and microscopy data collected in a subset of devices, however. We demonstrate that the electric fields dependency on the radius of a nanoscale conductive path can result in radial fields on the order of ~105-106 V/cm at only -1 V bias, sufficient to govern the negative resistive switching mechanism in filamentary devices. By accounting for this novel nanoscale size effect, long-standing anomalous experimental data about the negative (reset) resistance switching mechanism in bipolar filamentary resistive memory devices is finally reconciled. Full understanding of the switching mechanism predictively enabled additional control of the ReRAM RESET resulting in normal bipolar device operation coexisting with a 108 ON/OFF ratio unipolar switch which returns the device to the unformed state. Wide understanding of surface charges and associated radial electric fields will be important for future integrated circuit technology development and may enable new nanoscale technologies.

Automating CSR Aging Analysis for Organic Materials

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Compression stress relaxation experiments are important for studying aging and long-term mechanical performance in organic materials, but analysis workflows are often manual, difficult to reproduce, and tailored to specific datasets. This work presents an automated toolkit for processing accelerated-aging CSR data, estimating time-temperature shift factors, generating uncertainty-aware predictions, and producing auditable reports. The initial application was butyl O-ring aging analysis, but the workflow is designed to be adaptable to other organic materials and degradation studies.

The toolkit accepts raw experimental CSV files and metadata, standardizes preprocessing, identifies reference conditions, normalizes force-retention curves, and generates experiment-level plots. Material-level analysis groups experiments by material and temperature, estimates constrained horizontal shift factors, and fits Arrhenius-style relationships between shift factor and inverse temperature. Weighted linear regression plots provide a sensitivity check on room-temperature extrapolations and can help flag possible regime changes or changes in dominant aging mechanism.

An interface allows users to upload data, review experiments, run analysis, and download results without running any scripts directly. Outputs include processed data, experiment plots, shifted master curves, Arrhenius plots, prediction summaries, provenance information, and a self-contained HTML report. By centralizing preprocessing, analysis, uncertainty/sensitivity checks, and reporting, the toolkit improves reproducibility, usability, and auditability for CSR aging analysis.

From Slurry to Ceramic: Process Optimization for Fabricating MgO Ceramics with Vat Photopolymerization Additive Manufacturing

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Ongoing efforts seek to use projection-based vat photopolymerization additive manufacturing to fabricate magnesia parts for mission applications. However, there are several current challenges to manufacturing geometrically-complex, high-resolution ceramics, including the optimization of material development, print process parameters, and post-processing. A part development workflow is presented where parameters have been fine-tuned throughout every stage. Optimization starts at the powder system, where powder parameters are correlated with downstream firing parameters to develop formulations, which are iteratively refined to match rheological targets for printability. Part accuracy is also largely dictated by effective printer parameters. Correlating a printer's radiant light intensity to a resin's critical exposure level informs parameter selection for consistent curing across different printers. Leveraging these insights promotes higher chances of successfully fabricating robust ceramic parts.

High-Throughput Synthesis of High-Entropy Metal–Organic Frameworks for Chemical Warfare Agent Remediation

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High-entropy metal–organic frameworks (MOFs) offer a promising route to tune catalytic and hydrolytic activity through incorporation of multiple metals within a single node environment. However, MOF synthesis is often constrained by the complexity of multidimensional crystallization spaces and the continued reliance on manual, low-throughput experimentation. Here, we report an automated synthesis workflow for the rapid preparation and screening of mixed-metal MOFs based on UiO-66 and MOF-808 architectures for chemical warfare agent degradation. A robotic synthesis platform was used to automate reagent dispensing, heating, stirring, and parallel reaction execution, enabling reproducible and efficient exploration of synthesis conditions with reduced human error. Binary, ternary, quaternary, and quinary metal combinations were systematically investigated, yielding a range of multi-metallic framework compositions, including previously unreported materials. High-throughput powder X-ray diffraction (PXRD) was employed to rapidly assess crystallinity and phase formation, while preliminary energy-dispersive spectroscopy (EDS) was used to evaluate elemental composition and mixed-metal incorporation. This work establishes a foundation for discovering new high-entropy MOF compositions with potential for improved detoxification performance against chemical warfare agents and demonstrates how robotic synthesis can accelerate MOF discovery for catalytic remediation applications.

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Digital Fluid Modeling For Permanent Mold Hemispherical Castings of Aluminum Alloy with Varying Cooling Rates

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Several hemispherical cast products manufactured through a Gravity Die Casting (GDC) process from A-356 aluminum alloy were analyzed at different melt and mold pre-heat temperatures. The objective of this study is to determine the optimal thermal conditions through different cooling rates for a GDC process to obtain a high-quality cast with minimal defects. However, this process can be time and cost consuming, even for a widely used aluminum alloy such as A-356. Through the use of Computation Fluid Dynamics (CFD) software, such as FLOW-3D Cast and ANSYS Fluent, this process can be shortened, allowing for more efficient production cycles and higher quality products. A digital twin was modelled in FLOW-3D Cast to corroborate these results, which provides a reliable method to determine optimal thermal initial conditions.

Radiation tolerance of granular metal thin films

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This work evaluates the radiation tolerance of Mo-SiNx granular metals (GMs), composite materials composed of metal nanoparticles dispersed within an insulating matrix. The study of radiation-tolerant materials is relevant for medical devices and satellite electronics. The nonlinear impedance characteristics of GMs make them suitable for compact, high-efficiency passive snubbers and filters. The effects of equivalent electron fluence, total ionizing radiation (gamma), and displacement damage (N+ ions) were investigated. Devices maintained stable electrical properties up to 108 rad(Si) electron fluence, 1 Mrad(SiO2) gamma dose, and 1011 N+ ions/cm^2 displacement damage. Increasing the dose beyond these thresholds results in a steady decrease in resistance, which plateaus at approximately a tenfold reduction. Devices exhibited rapid annealing in air at ambient temperature, recovering electrical properties to within 10% of initial values over a time scale of several hours to several days. These results indicate that SiNx-based GM devices are suitable for use in radiation-sensitive fields such as space sciences and medical devices.

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Void Nucleation in an Oxide-Dispersion-Strengthened Copper Alloy

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The ductile failure of metals and alloys typically proceeds by void nucleation, growth, and coalescence. Current understanding of the specific mechanisms by which voids nucleate in undamaged material is limited, and knowledge of such processes has important implications for material models. Recent work has proposed that vacancies can condense into clusters that serve as void nuclei. This work examines that hypothesis by evaluating the effects of different initial vacancy concentrations and deformation rates on void nucleation in an oxide-dispersion-strengthened Cu alloy under uniaxial tension. Voids and surrounding microstructural features preserved from interrupted tension tests were characterized using various electron microscopy techniques. Voids nucleated primarily by debonding at the interfaces between oxide particles and the Cu matrix. Increasing the strain rate from 0.001 to 10 s^-1 had no significant effect on the density of voids formed. Specimens rapidly quenched from 1000 °C formed roughly twice as many voids per unit volume at a given strain as specimens cooled slowly from the same temperature in air. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Vibration and High Cycle Fatigue in Solder Joints

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Electronic components subjected to vibration environments can experience high-cycle fatigue in solder joints, ultimately leading to electrical failure. This work investigates vibration-induced fatigue damage in solder joints for several common surface-mount component types, including ceramic capacitors, SOT-26 gull-wing lead components, and ball grid array (BGA) packages. Test boards see single-axis vibration at 250 to 600 Hz on a vibration table while impedance is monitored in real time using time domain reflectometry. Changes in measured impedance are used to identify the onset of cracking. This enables the identification of vibration damage before an electrical open.

Following vibration testing, samples are cross sectioned to characterize crack initiation and propagation through the solder joints, metallization, and copper traces. In addition to conventional metallographic cross sections, serial sectioning using the Robo-Met system at Sandia National Laboratories is used to reconstruct three-dimensional crack paths through selected solder joints. These failure analysis methods provide insight into the relationship between component geometry, solder joint architecture, and fatigue damage evolution.

The experimental results are being used to calibrate and assess finite element analysis models of vibration-driven solder joint fatigue. By combining real-time electrical monitoring, failure analysis, and computational modeling, this work aims to improve prediction of time to failure across multiple electronic component types and package configurations. The resulting framework will support more reliable design and qualification of electronics exposed to dynamic mechanical environments.

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Advances in melt-based processing of aluminum alloys: Laser Beam Welding (LBW) & Wire Directed Energy Deposition (W-DED)

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Laser beam welding (LBW) and wire-directed energy deposition (W-DED) are single- and multi-pass melting processes used for joining and additive manufacturing, respectively. In dissimilar metal and alloy joining, LBW of aluminum alloy AA6061 to stainless steel alloy SS304L is complicated by differences in thermo-mechanical properties and the formation of brittle intermetallic compounds. To improve the fabrication of robust welds and enable additional dissimilar material combinations, the present study uses metallic interlayers deposited by a solid-state cold spray technique prior to LBW. Challenges to additive manufacturing of aluminum alloys include controlling microstructure while achieving desired properties, such as high strength, during rapid production of large-format stock. The W-DED technique enables rapid printing of high strength aluminum alloys with crack-free and equiaxed microstructures through a hybrid inoculant strategy.

Deep Learning-Based Segmentation for Porosity and Dendrite Quantification in Aluminum-Silicon Castings

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This study investigates the effect of processing conditions on the microstructure of aluminum silicon casting alloys using a deep learning pipeline. Solidification quality of samples is characterized and compared across preheating conditions and pouring temperatures. Microstructure analysis is quantified using a U-Net convolutional neural network to classify porosity and dendritic features, replacing manual and threshold-based methods that cannot reliably separate porosity from dendritic regions. This work analyzes the effects of processing parameters on pore formation, dendritic structure, secondary dendrite arm spacing, and grain size using features extracted from microstructural images. Porosity is measured as a function of height along the casting axis, and secondary dendrite arm spacing is correlated with measured cooling rate. By correlating processing parameters with porosity and dendritic microstructure, this work aims to clarify how processing factors influence pore and dendrite formation, supporting impurity-reduction studies that rely on porosity as an outcome measure.

High-Throughput Electrodeposition of Pt-Au Alloy Coatings Designed for Superior Wear Resistance in Electrical Contacts

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Tribological contacts are responsible for a large amount of global energy consumption (23%), prompting development of new and more efficient surface/lubrication materials to reduce energy costs via the reduction of tribological energetic waste. At Sandia National Laboratories (and beyond), several studies have shown nanocrystalline Pt–Au alloys have superior tribological properties in comparison with industry standard hard gold and other coatings. Despite these encouraging results, the Pt-Au alloy was only synthesized via physical vapor deposition (PVD), making it difficult to upscale to more complex surfaces or for use in industry. In this report, we detail an exploration into the various chemistries and conditions of the electrodeposition of Pt-Au alloys, as well as their corresponding structural and tribological properties. Our exploration of the individual and combined chemical/material space of both Pt and Au will be carried out via use of high-throughput infrastructure and techniques (electrodeposition and characterization) to elucidate ways to control the composition and properties of the targeted Pt-Au alloys. It will be shown that, with the right bath composition, electrodeposition can produce Pt–Au films with the same favorable coefficients of friction and wear rates as previously seen in the prior PVD studies, potentially opening the door for a more industrially ready technology (electroplating) to produce materials aimed toward the purpose of reducing tribologically-sourced energetic waste.

Sensitization and Recrystallization of AM Stainless Steel 316L under Repeated Annealing

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In this study, Laser Powder Bed Fusion Stainless Steel 316L (LPBF SS316L) is subjected to repeated thermal cycling up to 700 °C to determine its application on reusable casting molds and metal-metal composites. Two mechanisms were studied: sensitization and recrystallization. Both affect the steel's mechanical properties and corrosion resistance, which can alter the applicability of the additively manufactured (AM) steel. AM SS316L has a high hardness because of the internal stresses caused by rapid cooling, and it has anisotropy dependent on the build direction. To study microstructural evolution, multiple small samples were subjected to a 15-cycle thermal treatment, where each cycle consisted of sequential heating at 250 °C, 450 °C, and 700 °C with a 90-minute soak at each stage; cooled down by normalizing for 15 minutes and then quenching. Samples were analyzed at cycle intervals of 1, 3, 5, 10, 12 and 15 cycles, alongside an AM recrystallized control sample which was exposed to 1100 °C for 90 minutes then quenched. Etching, SEM, and EBSD techniques were used to analyze the sensitization development caused by precipitated carbides along the grain boundaries, and to study the advancement of recrystallization. EBSD data was post-processed using the MTEX toolbox for MATLAB to obtain maps and grain data which were used to observe the unique microstructural evolution of AM SS316L. The findings revealed that nano-oxides introduced into the steel by AM slowed down recrystallization by exerting pinning pressure on the grain boundaries. The steel then requires a higher annealing temperature or additional cycles to remove AM-induced characteristics like sub-granular dislocation structures, melt pools, internal strains, and grain morphology controlled by melt pool cooling. In terms of sensitization, the high presence of low angle grain boundaries from sub-grain boundaries and SS316L's low carbon composition suppressed the nucleation and growth of chromium carbides, although some localized sensitization was captured across all samples when focusing on grain boundaries. The hardness of the cycled samples was consistent across cycles; it was lower than the as-built condition but higher than the recrystallized control sample.

Infrared photoresponse and signatures of steady Floquet states in graphene systems

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Strong light-matter interaction in graphene induces Floquet-Bloch states, which may also have non-trivial topology [1–4]. We report on transport measurements of epitaxial graphene on SiC irradiated by a continuous-wave mid-infrared laser, using graphene Hall bars fabricated with a top gate that had high transmission in the mid-infrared range [5]. We observed signatures of a long-lived Floquet phase, where a non-equilibrium electronic population is stabilized by the interplay of coherent photoexcitation and incoherent cooling via phonon scattering. [6].

The capability to control the band structure by varying the twist angle in moiré lattices opens up a new way to explore light-matter interactions in these systems [7,8]. The occurrence of flat bands in magic-angle twisted bilayer graphene (MATBLG) leads to changes in the infrared photoresponse [9-12]. The photoresponse of MATBLG Hall bar devices reveals the complexity of the interplay between light and magnetic field in MATBLG systems, and opens up ways to further investigate the roles played by the substrate and the moiré potentials in the formation and stability of Floquet states.

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An ab initio molecular dynamics-based comparison of solute-induced stability of liquid-Al/intermetallic-Al3Sc interfaces

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Rare-earth element Scandium (Sc) is well-known for producing grain refinement in Al-alloys by forming intermetallic Al3Sc within liquid phase. The resulting low-energy liquid-Al/Al3Sc interfaces facilitate heterogeneous nucleation of face-centered cubic Al. However, deploying Sc at-scale is cost prohibitive, and motivates the search for alternatives that will reduce Sc content. Here, we have employed ab initio molecular dynamics to systematically interrogate the effect of ten solute substitutions on the thermodynamic and structural stability of the liquid-Al/Al3Sc interface at 1250 K: Zr, Ti, Ta, Nb, Li, Mg, Cu, Zn, Fe, and Ni. Their impact was quantified by computing Gibbs free energy, enthalpy of formation, excess interfacial free energy, and by probing variations in Bader charge and misfit strains. We found that Zr, Ti, Ta, and Nb were the most suitable substitutes, and resulted in measurably lower interfacial energies than the control. In contrast, Mg, Cu, Zn, Fe, and Ni were thermodynamically unfavorable, and the solutes demonstrated pronounced tendency to escape from their Sc-sites by migrating into the liquid phase. Crucially, these simulations permitted us to define a domain of stability for selecting potential elemental substitutions. It limits interfacial misfit strain to ~4% and Bader charge to ±1e, i.e, gaining or loosing at-most one electron from the surroundings. Together, our simulations provide a physical basis for designing light-weight Al-alloys that can reduce Sc content, while retaining its overall benefits.

Controlled formation of polyureas using microencapsulated isocyanate

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Polyureas (PURs) are soft polymer materials that possess exceptional properties upon deformation due to their phase separated microstructure and network of hydrogen bonds. In recent years, PURs have drawn significant interest as blast and impact mitigating materials due to their unique mechanical properties. The hindrance towards using PURs as functional materials is their high formation reactivity. PURs form upon mixing of isocyanates with amines and this formation can happen extremely fast, sometimes in seconds. Due to this, studies on PURs as impact mitigating materials are largely limited to films and coatings. It would be advantageous to reduce the formation reactivity of PURs to study their properties in bulk materials. Microencapsulation is a promising avenue towards reducing reactivity by encapsulating catalysts or monomers in a highly reactive system. In this work, we demonstrate that the isocyanate monomer can be encapsulated to protect the PUR reaction until a controlled external stimulus such as temperature is applied. PUR formulations developed with microcapsules are stable for an indefinite amount of time as shown in rheology, FTIR, and DSC studies. The mechanical properties of PURs formulated with microcapsules closely resemble those in non-encapsulated PURs. Finally, these microcapsule formulations can be 3D printed via extrusion to form bulk PUR structures for the first time. These 3D printed structures will be instrumental in studying functional PUR properties beyond films and coatings.

AI Assisted Discovery of High Entropy Alloys for Reversible Hydrogen Getters

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High Entropy Alloys (HEAs) provide a promising solution for hydrogen getter applications due to their tuneability and large hydrogen capacities. However, due to endless compositional possibilities, AI and ML models were implemented to readily discover novel alloy compositions that were thermodynamically tunable and highly hydrogen efficient. This work explores the fabrication and validation of these novel alloys and how they compare to their model predictions.

Investigating the Mechanism of Complete Conductive Filament Dissolution in Tantalum Oxide-Based RRAM Devices

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Metal-Insulator-Metal (MIM) resistive random-access memory (RRAM) switches by forming and rupturing nanoscale conductive filaments in the oxide (Larentis, 2012). Here we show that, after soft breakdown, TaOx RRAM can fully dissolve its conductive filament, restoring leakage to its pristine level, rather than merely constricting or partially rupturing it.

Earlier studies attribute reset to both field and thermally driven filament thinning, but never to full dissolution (Li, 2024). A reset device with a filament that is almost fully dissolved has similar semiconducting properties as high-k gate stacks used in traditional MOSFETs (Crepso-Yepes, 2010). The reset behavior also is very dependent on the material of not only the oxide but the electrodes as well (Wu, 2010). This behavior has also been theorized to be possible through Fick diffusion mechanics enhanced by the increased temperature inside the filament during the switching events (Valov, 2018), which is the mechanism we believe to be causing our empirical results. Therefore, with the correct material stack, bias conditions, and internal heating there exists a novel gap in understanding where complete filament dissolution should be possible in these metal-oxide based memory devices, which we have found working in our RRAM devices.

We combine I-V & C-V, low-frequency noise/random-telegraph measurements, and impedance spectroscopy to track forming, rupture, recovery, and dielectric changes. In-situ electroluminescence and bias-temperature mapping, combined with electrical data, correlate hot-spot emission to filament dissolution rather than vacancy redistribution. From these measurements our results reveal a temperature-driven dissolution regime in TaOx RRAM, given by characteristic patterns that go beyond simple reset behavior, and are characterized by the presence of complete filament dissolution. This dissolution regime offers a new mechanistic basis for endurance and recovery models and will guide the design of more reliable filamentary memories.

Resonance Engineering for Subwavelength Control of Light

Viktoriia Babicheva

UNM

Our work explores the engineering of electric and magnetic multipolar resonances in subwavelength dielectric nanoantennas for nanophotonic applications across the visible and near-infrared spectral ranges. By tailoring nanoantenna geometry, dimensions, and material composition, resonant modes can be precisely controlled to achieve strong electromagnetic-field confinement and manipulation at deep-subwavelength scales. High-refractive-index, low-loss dielectric materials enable spectrally tunable multipolar resonances while minimizing dissipative losses. Particular emphasis is placed on controlling the excitation and interference of multiple resonant modes to tailor the optical scattering response. By engineering the refractive-index contrast and nanoscale geometry, the interactions between electric and magnetic resonances can be precisely manipulated, enabling highly directional and, in particular, unidirectional scattering. These resonant phenomena provide a versatile platform for controlling light–matter interactions and offer opportunities for applications in optical sensing, imaging, and communications. The results demonstrate the potential of multipolar resonance engineering to provide precise control over nanoscale electromagnetic fields and far-field radiation, opening pathways toward advanced photonic devices with tailored optical functionality.
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Investigating Aqueous-Based Electrodeposition of Molybdenum for Use in Extreme Environments

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[1] SNL

Molybdenum (Mo), along with other refractory metals, are critical materials for advanced nuclear energy systems due to their exceptionally high-temperature strength and corrosion resistance. This study focuses on the electrodeposition of metallic Mo from water-in-salt electrolytes (WiSE) containing ammonium (NH4) and potassium (K) acetate, a promising approach for fabricating high-quality coatings tailored for fission or fusion reactor applications. Despite historical research on acetate-based electrolytes for Mo electrodeposition, the fundamental roles of electrolyte constituents and their influence on deposition mechanisms and outcomes remain unclear. To address this, we investigated the effects of key variables, including water-to-salt ratio, NH4/K ion ratio, temperature, pH, and current density on the electrodeposition process using (NH4)2MoO4 containing WiSE. We identified a minimum NH4+ fraction threshold above which metallic Mo deposition is activated, resulting in films of metallic Mo. The extent of oxide formation (i.e. fraction of metallic Mo vs. molybdenum oxides) was evaluated via energy-dispersive x-ray spectroscopy and x-ray diffraction analysis, as pure Mo is essential for protective coatings on reactor components.

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Improving Solder Joint Strength in AM Flex Cables

Joshua Minster[1], Hannah Fowler[1], Emily Huntley[1], Steven DiGregorio[1]

[1] SNL

Additively manufactured (AM) flex cables enable rapid, customized electronic interconnects, but reliable surface-mount (SM) solder attachment has been limited by weak adhesion between inkjet-printed silver pads and acrylate substrates. Prior plated-through-hole (PTH) geometries performed well, showing strong solder pull strengths and favorable fractography. In contrast, earlier SM samples exhibited pad delamination at the Ag/acrylate interface, motivating this effort to improve SM pad adhesion through mechanical anchoring.

Mechanical anchoring features were incorporated into SM pad designs and evaluated using IPC-style 9-spot pin pull testing. Anchor diameter and spacing were varied relative to an unanchored control. Mean pull strength increased monotonically with anchor packing density, with the highest-density designs achieving approximately 2.6"-" 2.8× the control mean strength. Failure mode shifted from Ag/acrylate interfacial delamination to mixed-mode failure within the anchored pad/substrate system, indicating improved interfacial integrity under load.

These results show that mechanical anchoring is an effective strategy for increasing SM joint strength in AM flex interconnects. Ongoing work includes further optimization of anchoring strategies to extend reliability across application environments and evaluation of various coupon geometries (BGA).

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

An Ab Initio Molecular Dynamics study on water confinement in Quartz

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Water is known to influence the slow weakening and failure of silica-based materials, but the behavior of water confined within quartz with narrow openings is still not fully understood at the atomic scale. In this study, ab initio molecular dynamics simulations were used to examine the effect of water confinement on the structural, mechanical, and chemical response of hydroxylated quartz with an aperture of 3.6Å. Three water-populated systems containing 1, 8, and 10 H2O molecules were simulated in the NVT ensemble at 300K for 50 picoseconds.

We found that hydrogen bonding behavior changed as the number of water molecules increased. The three systems developed from a surface-dominated interaction at low hydration level to a more connected hydrogen bond network at higher hydration levels within the aperture. Due to the interactions between hydrogen bonds and surface OH-SiO bonds, deformation was focused around the quartz-water interface. This resulted in a greater aperture opening with the mean separation between the opposing quartz surface layers being 4.4Å for the 1-H2O system, 5.6Å for 8-H2O and 5.9Å for 10-H2O systems. Despite these changes, the average Si-O bond length remained intact in all three systems, indicating no bond-breaking to the quartz network for the 10,000 iterations simulated. Overall, these findings provide atomistic understanding into processes that may occur before water-assisted weakening and fracture of silica.

Computational screening of amino acids for trapping rare-earth elements in aqueous solution using AIMD and tight-binding principles

Brianne Boyd[1], Deep Choudhuri[1], N. Scott Bobbitt[2], Dorina Sava Gallis[2]

[1] NMT; [2] Sandia

This study aims to screen a large number of generated rare earth element-amine complexes for binding affinity with tight binding methods as well as ab initio Molecular Dynamics (AIMD) . Since rare earth elements are uniquely difficult to separate due to their complex electronic orbital behavior, finding amino acids that prefer one REE over another may be incredibly valuable. By implementing a combination of tight binding methods and AIMD, this study both screens a large number of complexes for affinity and computationally tests promising conformers at temperature. Structures were generated using the Los Alamos created Architector, a high-throughput tight-binding based software that builds and relaxes realistic f-block complexes using built in parameters specific to the lanthanide series. Screening of the amines glycine, aspartic, and histidine, as well as combinations thereof, show that a histidine-aspartic combination has greater affinity for both Nd and Ce than the other amines. Computed 0K interaction energies of this combination show a preference for Ce over Nd. AIMD testing at 300K corroborated these results. This workflow enables rapid screening of amine selectivity, potentially saving valuable time and resources during REE separation efforts by identifying promisingly selective amino acids for experimentation

Comparison of the tensile deformation behavior of BCC+B2 and HCP+B2 microstructures in a Zr-Ru refractory alloy

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Ru-containing refractory alloys provide an excellent pathway for developing BCC+B2 microstructures to achieve good high temperature performance. However, the effect of Ru on the temperature dependent deformation behavior of refractory metals is not well understood. Our previous study on the phase stability of a Zr80Ru20 alloy indicated that the alloy transforms from BCC+B2 to HCP+B2 when annealed at 600 °C. This provides an opportunity to investigate the deformation behavior of BCC and HCP matrices with different Ru solubility. Tensile tests of these two microstructures have been conducted at 200 °C, 400 °C, 600 °C, and 800 °C, and results showed that BCC+B2 is stronger but also more ductile than HCP+B2. To further understand the deformation behavior of BCC+B2 and HCP+B2, partially strained and failed samples were examined using transmission electron microscopy.

Constitutive Calibration as a Data Problem: Physics-Informed Machine Learning using High-Rate Experiments on an Ontology-Backed Workflow

Erwin Cazares[1], Brian E Schuster[1]

[1] The University of Texas at El Paso

Calibrating a flow-stress model from mechanical tests is a data-centric problem. With a Split-Hopkinson campaign spanning only a few dozen stress-strain curves, the classical least-squares approach cannot separate correlated parameters, says nothing about the response between tested rates, and estimates uncertainty only after the fit. We present a physics-informed calibration architecture that co-trains a flexible neural surrogate with the constrained constitutive law. The two are coupled to experimental data and to collocation points where no test was run, and an ensemble of independent fits directly reports parameter uncertainty. A model-agnostic core treats each law as data, so two laws of contrasting origins can be calibrated through a single pipeline: the empirical Johnson-Cook law and the dislocation-based Zerilli-Armstrong law. We validate the stress-surface tool and material card parameters by comparing the simulated specimen response with measured curves across the full rate range. We paired the following architecture with an ontology-based GUI for high-rate methodologies, reduction of the experimental data, training of machine learning algorithms, and provenance tracking according to the FAIR methodologies

Grain Size and Temperature Effects on Twinning and Slip in ECAP-Processed WE43 Magnesium Alloy

Andres Maldonado[1]

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A major challenge in WE43 is understanding how the rare-earth alloyed elements modify deformation behavior in response to changes in grain size and temperature. Magnesium alloys have been at the leading forefront for the development of high strength to weight ratio materials but are limited by their hexagonal closed-packed (HCP) crystal system. This restricts the number of activated slip systems therefore, resulting in a reduction of plastic deformation and ductility. Procedures such as severe plastic deformation (SPD) have been used to overcome these obstacles by promoting grain size refinement, improving material strength, and increasing formability. Equal-channel angular pressing (ECAP), a specified SPD technique, uses an angled channel to impose elevated temperatures and pressures on the material. In this experiment, WE43 was processed through ECAP to investigate the influence of severe plastic deformation and its effects on material behavior across various temperature conditions. Subsequently, the relationships between grain size, crystallographic texture, and the deformation mechanisms such as slip and twinning were compared. Small-scale mechanical testing was performed over a range of temperatures to evaluate the effects of grain size and temperatures on twinning and dislocation slip. This was characterized by backscatter diffraction (EBSD), a method used to analyze microstructure and texture evolution to provide evidence of activated twinning and dislocation slip in both coarse and ultrafine grained WE43. Therefore, by comparing these conditions, this study aims to determine how ECAP induced grain refinement influences both twin activation and dislocation slip during deformation.

Screening Amino Acid Rare Earth Complexes for Selective Binding Using Tight-Binding Methods and AIMD

Brianne Boyd[1], N. Scott Bobbitt[2], Dorina F Sava Gallis[2], Deep Choudhuri[1]

[1] NMT; [2] Sandia

Rare-earth elements (REEs) are challenging to separate because of their similar ionic radii and complex electronic structures, motivating the search for ligands or combinations of ligands that can selectively bind one REE over another. In this study, we computationally screened REE-amino acid complexes in aqueous environments to evaluate binding affinity and selectivity using a workflow that combines tight-binding methods, as well as ab initio Molecular Dynamics (AIMD). Candidate structures were generated using Architector, a high-throughput tight-binding based software that builds and relaxes realistic f-block complexes using built-in parameters specific to the lanthanide series. We examined glycine, aspartic acid, histidine, and combinations of these amino acids at 0 Kelvin as ligands for La, Ce, Nd, Gd, and Dy. Initial screening identified histidine-aspartic acid complexes as having stronger affinity for all lanthanides considered) than the other amino acid systems that were studied. Also we find evidence of synergistic binding effects between histidine and aspartic acid, resulting in binding affinity greater than the sum of their parts. Computed 0K interaction energies of this combination indicate a preference for Ce over Nd for this ligand configuration. Due to resource constraints, AIMD testing was limited to Ce and Nd, which corroborated these results. Overall, this workflow enables rapid screening of favorable amino acids-REE complexes, helping prioritize selective ligand candidates for experimental validation relevant for several REE separation techniques.

This work is supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND2026-26111A

Strain State – Strain Rate – Temperature Interplays in Tensile Failure of Pure Tantalum

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Tantalum is a refractory metal with excellent elevated-temperature strength, acceptable weldability and formability, and superb corrosion resistance, making it ideal for demanding power generation and chemical processing applications. As a body-centered cubic metal, pure Tantalum (Ta) is known to exhibit thermally activated dislocation slip, which causes strong temperature and strain rate dependence on flow strength. However, interplays between temperature and strain rate have only been reported in thick-section bar stock and less is understood about failure in thin sheets. Here, we explore strain rate-temperature-strain state interplays in commercially available wrought pure Tantalum. The constitutive properties (strain rate & temperature) and effect of geometric constraint (strain state within a notch) on fracture in tension is evaluated between 22 and 900 °C.

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Compression vs. Tension-Induced Wrinkle Formation on Thin Film Structures: Three-Dimensional Numerical Simulations

Md Al Rifat Anan[1], Donghyeon Ryu[2], Yu-Lin Shen[1]

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The development of surface wrinkles on thin films bonded to compliant substrates is recognized as a form of mechanical instability. While this wrinkling behavior is widely studied when the thin film is under direct compression, much less attention has been devoted to the prediction of wrinkle formation caused by tension and cyclic compression-tension deformations. This work focuses on compression vs. tension-induced wrinkles using a relatively stiff polymeric film on an elastomeric substrate as the model system. Experimental observations show that parallel wrinkles formed during unidirectional compression gradually disappear under reverse loading. When the thin film structure is pulled into tension, a new set of parallel wrinkles in the perpendicular direction would develop. The tension-induced wrinkles are caused by Poisson's ratio mismatch between the film and substrate, which generates lateral compression in the film. By way of the embedded imperfection technique in three-dimensional (3D) finite element modeling, we illustrate that this type of wrinkle transition can be simulated in a seamless manner. With the linear elastic assumption, the overall load-displacement response and evolution of wrinkles are shown to be reversible. The tension-after-compression and direct tension loading conditions lead to exactly the same material response, including the deformation instability. Further analyses on the effects of film modulus and Poisson's ratio are performed, with the differences in wrinkling behavior under compressive and tensile loading contrasted.

Femtosecond Laser Machining of Site-Specific Micromechanical Test Samples for Interfacial Property Characterization

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Site-specific micromechanical sample fabrication is a rapidly expanding field of study that seeks to extract materials properties in the micro scale within a specific region of interest. Much work in this field relies on micro to nanoscale sample fabrication using a focused-ion beam, while millimeter to micron-sized samples are typically produced using wire-EDM. This work establishes a method to mill site-specific micromechanical samples using a femtosecond laser system, achieving a high-throughput methodology that outpaces focused-ion beam in the micron scale while inducing less material damage into the samples than Wire-EDM in the millimeter scale. Using the femtosecond laser system, we mill site-specific micromechanical testing specimens from both matrices and the interface in an explosively-welded aluminum-titanium bimetallic. We also use the laser capabilities to cut site-specific tensile samples targeting microstructural twins in ultra-high purity macro-grained nickel samples. We test these samples in-house using a micromechanical testing stage to generate interfacial materials property data at both the explosive welding interface and the interface of the twin boundaries. Results demonstrate that femtosecond laser machining successfully bridges the gap between focused-ion beam and wire-EDM, yielding micromechanical specimens with minimal heat-affected zones and processing times much quicker than FIB.

A dual method approach to development of printable age-hardened Al-Cu alloys for LPBF applications

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[1] New Mexico Tech

The rapid solidification seen in laser powder bed fusion (LPBF) and other types of additive manufacturing causes issues with segregation and solidification cracking especially in aluminum copper alloys. The ubiquitousness of Al-Cu alloys in engineering applications and the advantages of additive manufacturing makes research and development of alloys that print well of paramount importance. Previous research has demonstrated that grain refinement can improve printability as well as serving to increase alloy strength. Cracking can be mitigated by increasing the amount of liquid present during final solidification via addition of eutectic forming elements. This work will show that alloying Al-Cu with grain refining elements such as Zr and Ti and eutectic forming elements such as Si can greatly improve the printability of as well as produce mechanical properties approaching Al-2024. Printability is assessed via SEM, EDS, and EBSD. Tensile strength is measured using printed tensile bars.

Atomistic Insights into Solid-Melt Interfacial Properties and Dendrite Orientation Transition in Al-Mg-Zn Alloys

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Solid-melt interfacial free energy and its crystalline anisotropy are fundamental thermodynamic parameters that govern dendrite growth direction and morphology, ultimately dictating the texture and mechanical properties of the cast. While previous atomistic studies have largely focused on simple binary systems, commercial aluminum alloys are inherently multicomponent. Accurately predicting microstructures in these alloys requires a deep understanding of the complex solute-solute and solvent-solute interactions, studies for which is limited. To bridge this gap, we employ Molecular Dynamics (MD) combined with the Capillary Fluctuation Method (CFM) and Semi-Grand Canonical Monte Carlo (SGCMC) simulations to investigate equilibrium solidification in the ternary Al-Mg-Zn system. We demonstrate that progressively replacing Mg with Zn shifts the preferred primary dendrite growth orientation from the conventional <100> direction to a hyperbranched regime, which is marked macroscopically by feathery grains. This transition is driven by a combined atomic size mismatch and chemical affinity mismatch between the solvent and solute atoms. Furthermore, while the interfacial free energy remains relatively stable across alloy compositions, it is slightly elevated in Zn-rich ternary compositions. We link this increase to Chemical Short-Range Ordering (CSRO) and solute clustering between solute atoms within the in-liquid ordered zone adjacent to the interface. Ultimately, this study reveals how solute-solute interactions can modulate interfacial properties, offering a practical pathway to achieve alternate dendrite growth directions and textures purely by tuning the alloy chemistry.

Nanoscale Structural and Compositional Evolution of Mo-SiNx and Fe-SiNx Granular Metal Thin Films

Teagan Della Cerra[1], Simeon Gilbert[2], Darryl Shima[1], Laura Biedermann[2], Ganesh Balakrishnan[1]

[1] University of New Mexico; [2] Sandia National Laboratories

Granular metals (GMs) are metal nanoparticles suspended in a dielectric. Their electrical, optical, and magnetic properties can be tailored through deposition and post-processing. Charge transport occurs through electron tunneling at low frequencies and capacitive coupling at high frequencies, making properties dependent on nanoparticle (NP) size, distribution, and interfacial chemistry [1]. Understanding how annealing affects GM nanostructure is important for optoelectronic, extreme-environment, conductive, and magnetic applications [2-4]. In Mo-SiNx GMs, defect control and larger, more widely spaced NPs suppress low-frequency resistive transport while preserving high-frequency conductivity [5,6]. We are investigating Mo-SiNx films for nanosecond-responsive shunt devices and Fe-SiNx films for magnetic inductor cores. We examine radio-frequency-sputtered Mo-SiNx and Fe-SiNx GMs using complementary electron microscopy techniques. Scanning electron microscopy (SEM) evaluates surface morphology, while focused ion beam (FIB) preparation enables site-specific cross-sectional transmission electron microscopy (TEM) and selected-area electron diffraction (SAED). These methods assess grain size, distribution, structure, and phase. Energy-dispersive X-ray spectroscopy (EDS) mapping and line scans examine elemental distribution, metal segregation, and annealing-induced compositional changes. Comparisons of as-deposited and annealed samples reveal differences in grain coarsening, phase contrast, and metal-matrix connectivity between the systems.

Correlated SEM, EDS, FIB, and TEM analysis links processing conditions to nanoscale structure. Clarifying grain evolution and elemental redistribution during annealing advances the understanding of structure-property relationships and informs the design of tunable electronic, magnetic, and photonic materials.

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Computational Analyses of Effective Elastic Modulus and Thermal Conductivity of Porous Structures from Closed-cells to Open-cells

Ushnik Ghosh[1], Yu-Lin Shen[2]

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This paper presents a systematic numerical investigation of the effective elastic modulus and thermal conductivity of porous materials across the full porosity range, from closed-cell to open-cell configurations. Three-dimensional finite element models are developed using a periodic unit-cell approach, along with idealized “all closed-cell” and “all open-cell” geometries to isolate the effects of phase connectivity. The simulations show that the effective elastic behavior is highly sensitive to pore geometry and connectivity, with the response of generic porous structures falling between the idealized bounds at low porosity but deviating at higher porosity. In contrast, the effective thermal conductivity generally lies between the closed-cell (upper) and open-cell (lower) bounds, with a discernible transition near the percolation threshold. These findings clarify how pore connectivity governs mechanical and thermal performance in porous solids, with implications for biomimetic design and engineered cellular materials.

Computational Analyses of Effective Elastic Modulus and Thermal Conductivity of Porous Structures from Closed-cells to Open-cells

Dennis Robinson Brown, David Montes de Oca Zapiain, Tina Nenoff, Jessica Rimsza

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Porous liquids (PLs) are a class of liquids and colloids with permanent internal porosity for selective gas sorption. Often, PLs are composed of porous nanoparticle sorbents like metal organic frameworks (MOFs) suspended in a sterically or chemically excluded solvent. Such PLs are classified as Type 3 and have demonstrated emergent high gas uptake that can exceed that of the individual constituent solvent or sorbent material. Until recently, materials design for PLs has relied on broad heuristics and a trial-and-error approach to discover novel compositions with high selectivity. For instance, PL solvents are often proposed using crude point estimates of solvent molecular size (e.g., van der Waals radii) in comparison to the sorbent pore window size. In more recent studies, empirical forcefields have enabled molecular metrics of solvent-sorbent size compatibility. By leveraging existing databases of MOF gas sorption data and advanced solvent screening procedures, PL development timelines can be profoundly accelerated.

Here, we leverage web scraping, cheminformatics, and large language models (LLMs) to streamline the discovery of novel PL compositions with emergent CO2-selectivity for biogas separations applications. The lightweight version of Metaâ€™s Llama 3.2 with one billion parameters was trained on the hypothetical MOF (hMOF) database using the low-rank adaptation (LORA) fine-tuning approach to predict the utility of a given MOF for biogas separations. Specifically, MOFs with predicted CO2/CH4 selectivity greater than 5 were deemed industrially viable to scrub CO2 from biogas. Then, a set of 90,000 solvent molecules were autonomously scraped from PubChemÂ®. A Python-based cheminformatics library (RDKit) was used to rapidly estimate the radius of gyration distribution, P(Rg), for the proposed solvents. By searching for solvents with minimal overlap between P(Rg) and MOF pore window size (the pore limiting diameter), the possible solvents were reduced from tens of thousands to hundreds of candidate solvents. Further solvent down-select used solvent properties (e.g., boiling and melting point temperatures) to generate an experimentally testable set of tens of solvent-sorbent pairs. This high-throughput in silico materials discovery workflow will accelerate materials discovery for PLs with emergent gas separations potential and commercial viability. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Expanding the Materials Toolbox for Vat Photopolymerization

Hayden Fowler[1], Meghan Kiker[1], Samuel Leguizamon[2], Savannah River National Laboratory; Leah Appelhans[1], Yuval Vidavsky[3], Hailey Bates[1], Johanna Vandenbrande[4], Ryan Hensleigh[4]; Johanna Schwartz[4]

[1] Sandia National Laboratories, [2] Savannah River National Laboratory, [3] Soreq Nuclear Research Center, [4] Lawrence Livermore National Laboratory

The increasing complexity of next-generation components demands advanced materials and manufacturing techniques that enable agile production with modularity and precision. These components require stringent performance criteria such as tight dimensional tolerances, customized compression and tensile loading profiles, frequency-specific shock and vibration mitigation, and significant weight reduction while maintaining high static or dynamic load-bearing capacity. Vat photopolymerization, an additive manufacturing process that selectively cures liquid resin to produce high-resolution 3D parts, offers a promising route to meet these challenges with design flexibility. However, the predominant reliance on acrylate photopolymerization has constrained the diversity of materials properties achievable through vat photopolymerization. Here, we investigate alternative chemistries, specifically those enabled by transition metal catalysts, to broaden the spectrum of materials properties and enable unique functionalities. We demonstrate vat photopolymerization with photoinitiated ring-opening metathesis polymerization (photoROMP) for additive manufacturing of a diverse array of polyolefin materials, including tough thermosets, semicrystalline thermoplastics, and flexible elastomers. We further demonstrate vat photopolymerization of silicones via platinum catalyzed hydrosilylation with tunable lattice structures for targeted compression profiles.

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Expanding the Materials Toolbox for Vat Photopolymerization

Thiagarajan Soundappan

Navajo Technical University

Limited resources and access to centralized healthcare facilities within the Navajo Nation have underscored the urgent need for low-cost, decentralized diagnostic tools. This talk presents the NEST Labâ€™s work on the simple and scalable fabrication of paper-based and laser-induced graphene electrodes for electrochemical sensing and biosensing applications. These platforms enable the sensitive and selective detection of heavy metals, biomolecules, clinically relevant cancer biomarkers, and bisphenol (BP) compounds, an important class of endocrine disruptors linked to environmental and health concerns. Using accessible techniques such as hand coating, wax patterning with a commercial wax printer, and laser engraving, we have engineered sensors that are affordable, portable, and well-suited for deployment in underserved and remote areas. The NEST Labâ€™s research also provides valuable training opportunities for undergraduate students at Navajo Technical University, offering hands-on experience in electrochemical research, sensor design, fabrication, and testing. Through this work, Navajo students are empowered to address real-world challenges in their communities, including water contamination, exposure to endocrine disruptors, and early disease detection, thereby helping bridge the gap between advanced research, STEM education, and meaningful local impact within the Navajo Nation.

Performing a Solar Oberth Maneuver to Reach the Near Interstellar Medium with a Solar Thermal Propulsion System

Jason J. Benkoski[1], W. Lloyd Luedeman[2], James P. Mastandrea[2], Jessica Harsono[2], Narendra N. De[2], Michael C. Brupbacher[2], Michael Presley[2], David M. Deglau[2], Joseph Scroggins[2], Mark W. Buchta[2], Dajie Zhang[2], Michael E. Thomas[2], Gabriella M. Hunt[2], Ryan H. Carter[2], Joshua D Mitchell[2],H. Dave DeMarsh[2], Ralph McNutt[2], Pontus C. Brandt[2],Michael V. Paul[2]

[1] LANL, [2] JHU/APL

The feasibility of an interstellar mission hinges on the ability to achieve a high escape velocity. 20 AU/yr would be required to reach 500 AU approximately 25 years after launch. Such speeds may be possible by performing a powered gravity assist around the Sun. We are developing an unconventional approach that simultaneously addresses the need for high specific impulse and close proximity to the Sunâ€“convert the heat of the Sun into usable thrust by passing a propellant through the heat shield.

To demonstrate the efficiency of solar thermal propulsion at the benchtop scale, we designed and fabricated a 20 x 20 cm solar thermal propulsion prototype. The reflective yttria-stabilized zirconia (YSZ) coating and helium gas flow combined to maintain a temperature of 66Â°C during illumination by 20 Suns equivalent intensity. With a dark chrome oxide coating facing the solar simulator, the system could generate a thrust of 1.3 N at a flow rate of 0.6 g/s and a temperature of 243Â°C. Having validated the model at low temperature, we now have a theoretical model in place to more confidently predict performance at high temperature, once the high temperature properties of the materials are known with greater certainty.

Expanding the Materials Toolbox for Vat Photopolymerization

Kendall Yetter[1], Michael Lester[1], Michael Sangid[2], William LePage[1]

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This work presents a new way to smooth rough surfaces without material removal, as well as heal cracks in metals. Both approaches utilize transient liquid phase surface metallurgy. Rough surfaces are often the cause of fatigue failures in additive parts. Therefore, surfaces are typically treated by etching and/or abrasive techniques. These existing techniques require material removal, which must be compensated by over-building. To smooth surfaces without material removal, our new transient liquid phase approach smooths metal surfaces and can also impart compressive residual stress and/or hardness enhancements. The operation of transient liquid phase smoothing is two steps: coat the part with a eutectic-forming film, and then heat treat the part to activate local surface melting (ideally with a heat treatment step that would be performed already, such as a stress-relief). In addition to smoothing surfaces and imparting compressive residual stress, transient liquid phase surface metallurgy can heal cracks with a similar approach. This presentation will share results from both surface smoothing and crack healing, with an emphasis on connecting the overall performance to the underlying process and structure.

Nuclear fuel performance simulations of gas evolution, swelling and creep informed by lower length scale investigations

David Andersson

Los Alamos National Laboratory

Fission gas evolution, swelling and creep in nuclear fuels are controlled by atomic scale diffusion processes that are governed by the chemistry of the fuel, temperature, and irradiation conditions. In order to facilitate accelerated qualification of new fuel types, mechanistic models have been developed for these processes in several fuel types, e.g. UO_2 and UN. This was accomplished by first investigating atomic scale defects and diffusion processes using density functional theory (DFT) and empirical potential calculations. The results of these calculations are then used to parametrize cluster dynamics models describing the response to irradiation. Finally, the gas evolution, swelling and creep rates are captured by use of the rates predicted by cluster dynamics simulations in model equations governing the macro-scale response of the fuel pellet. The engineering scale fuel pellet behavior is predicted by the BISON fuel performance code. This approach will be showcased by select examples for UO_2 and UN. Both the lower length scale and engineering scale predictions for these two fuel types are compared to available experimental data. To demonstrate the ability to reduce uncertainties of the mechanistic models, a Bayesian framework was developed to calibrate the model to experimental data for UO_2 and UN.

Poster Presentations

Closed-Loop Robotic Electrodeposition for AI-Accelerated Materials Processing

Spencer Newman[1], Jason Taylor[1], Matthew Roop[1], Tylan Watkins[1], Ryan Katona[1]

[1] Sandia National Labs

Autonomous experimentation can accelerate materials process development by replacing manual trial-and-error workflows with data-driven, closed-loop control. In electrodeposition, achieving a target coating thickness often requires iterative tuning as deposition efficiency varies with sample condition, electrolyte chemistry, temperature, and operating parameters. We developed an automated electrodeposition platform that integrates robotic sample handling, electrochemical control, analytical mass measurement, and probabilistic machine learning to learn and execute thickness-targeted deposition. The platform uses a Mecademic Meca500 six-axis robot, a BioLogic SP-300 potentiostat, and a Mettler Toledo analytical balance under Python-based control. For each experiment, the system weighs a sample, performs electrodeposition at a selected current and duration, reweighs the sample, and estimates coating thickness from the measured mass change. If the measured thickness is below the target, the workflow autonomously selects and performs an additional deposition step while recording process conditions and outcomes. Experimental data are used to update a probabilistic machine learning model that predicts the deposition time required to achieve a specified thickness, including uncertainty in the deposition response. Over repeated trials, the system improves its predictions and reduces the need for operator intervention. This work demonstrates a self-improving materials processing workflow that combines robotics and machine learning to improve reproducibility and efficiency in electrochemical coating fabrication, highlighting a broader path toward AI-accelerated materials development.

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Printability of Particle-Laden Inks

Carlos Zubeldia[1], Emma Joly[1], Lucas Raymond[1], Joseph Monti[1], Jess Kopatz[1], Rekha Rao[1], Dan Bolintineanu[1], Harrison Root[1], Hayden Fowler[1]

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Printability of Particle-Laden Inks Direct Ink Write is an additive manufacturing technique in which ink is extruded through a syringe nozzle onto a substrate. DIW inks are shear thinning, yield stress fluids composed of a liquid base and solid filler, behaving as a fluid during extrusion and as a solid after extrusion. They are characterized by their adherence to this property as either runny, printable, or jammed. Previous work has shown that the best indicator of the printability regime for a given ink formulation is the maximum filler particle packing fraction, which can be predicted using particle morphology.

This research combines computational modeling and experimental testing to reduce the workload needed to determine printability. First, particle morphologies for several filler materials were characterized. Leveraging characterization data directly, LAMMPS discrete element method simulations were performed to determine the maximum packing fractions for size-bimodal particle mixtures. In parallel, Goma finite element method simulations were used to quantify particle migration and die swell during extrusion for several filler materials. Finally, an empirical model from the literature was employed to estimate the maximum packing fraction and identify the printability regime, providing a basis for calibration and comparison with the particle packing model.

Goma simulation results show that particle migration is positively correlated with particle size and negatively correlated with volume fraction, and vice versa for die swell. Further, the diffusive flux model reflected larger die swell but less particle migration than the suspension balance model. The LAMMPS packing model agreed with the empirical packing model to varying degrees for different materials. Lastly, extrudability and DIW tests were performed on inks informed by empirical model calculations. The experimentally determined printability regime differed from the volume fraction of extrudable inks, and some extrudable inks were not printable.

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Sodium Ion Transport Behavior in Ta, Mg, Zn-Doped NaSICON

Cameron Martin[1], Isaac Dyer[1], Amanda Peretti[2], Leo Small[1]

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Increasing the ionic conductivity and sodiophilicity of the sodium (Na) Super Ion CONductor (NaSICON) can improve the performance of sodium-based batteries by lowering interfacial resistances and increasing energy efficiency. Specific dopants are theorized to enhance ion movement by altering the crystal structure and lowering the activation energy for Na+ transport. This study aims to investigate how Ta, Mg, and Zn-doping on the Zr site of NaSICON ($Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$) affects the microstructure and ionic conductivity. NaSICON samples were synthesized with 0.05-0.2 moles Ta, Mg, and/or Zn per formula unit and characterized via density measurements, scanning electron microscopy (SEM), x-ray diffraction (XRD), and electrochemical impedance spectroscopy (EIS) from 50°C to -70°C for conductivity and activation energy analysis. All samples displayed densities of at least 97%, and Ta-doped samples showed a slight increase in formula mass, suggesting a possible increase in density. Mg-doping increased ionic conductivity at room temperature from 3.74 to 4.71 $mS \cdot cm^{-1}$ and reduced total activation energy from 0.312 ± 0.005 eV to 0.299 ± 0.005 eV to promote fast charging through Na+ ion movement. Differences in microstructure from SEM and crystal structure from XRD will be related to dopants present. The potential of individual or a combination of dopants in NaSICON to enhance the ion transport and microstructure promises safe, long-lasting sodium batteries for the future.

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Tannic Acid Loaded MgO and ZnO Doped Antibacterial Hydroxyapatite for Orthopedic and Dental Applications

Claire Putelli[1], Joel Pilli[2], Gwenever Gatto[2], Arjak Bhattacharjee[1]

[1] Materials Metallurgical Engineering, New Mexico Institute of Mining & Technology; [2] Biology, New Mexico Institute of Mining & Technology

This study addressed the critical challenge of post-surgical bacterial infections, specifically osteomyelitis, associated with traditional hydroxyapatite (HA) bone grafts. A novel, multifunctional scaffold was developed by co-doping HA with magnesium oxide (MgO) and zinc oxide (ZnO) and incorporated plant-derived tannic acid (TA). Experimental results demonstrate that these co-doped, TA-loaded scaffolds maintained structural integrity and cytocompatibility while achieving approximately 94% antibacterial efficacy against Staphylococcus aureus. This approach offers a promising, non-cytotoxic alternative for orthopedic and dental bone reconstruction, leveraging the synergistic antibacterial effects of the metal oxide dopants and the natural medicinal properties of tannic acid.

Impact of Tantalum Oxide Layers on Two-Color Pyrometer Readings

Trace McKissack[1], Brian Schuster[1]

[1] University of Texas at El Paso

Tantalum crucibles are often used in laboratory and industrial applications due to tantalum's high melting point and corrosion resistance. The crucibles can be heated in air to produce an oxide layer that reduces adhesion between the crucible and any material within. Two-color pyrometers are often used to measure the temperature of the crucible during the heating process. Two-color pyrometers measure thermal radiation emitted by the sample at two wavelength bands to determine temperature. The oxide layer on the surface of the tantalum crucible changes how thermal radiation is emitted from the crucible. The purpose of this research is to determine how the oxide layers affect temperature readings from the two-color pyrometer. This will be achieved by preparing multiple tantalum samples with differing thicknesses of tantalum oxide and determining how this affects the thermal radiation emitted.

Time-Dependent Effects of Hydrogenation and Dehydrogenation on the Mechanical Behavior of Ti-6Al-4V

Cesar Valle[1], Brandon Cepeda[1], Andres Maldonado[1]

[1] UTEP

This study investigates the time-dependent hydrogenation and dehydrogenation behavior of Ti-6Al-4V alloy on microstructural development and mechanical behavior. Hydrogenation treatments of different duration times were used to evaluate β-phase stabilization, and potential hydride formation, as hydrogen acts as a temporary alloying element which stabilizes the β phase, lowering the α→β transformation temperature. Dehydrogenation was performed under inert conditions to remove hydrogen while retaining microstructural changes. To characterize the phases of the material during the treatment, XRD was used, while metallography and EBSD were employed to characterize microstructure. Results show that hydrogen exposure time influence phase and microstructure, which affects hardness after dehydrogenation.

Photoelectric Work Function Measurements of Potassium Doped HOPG

Richard Shulyak[1], New Mexico Tech[1]

[1] New Mexico Institute of Mining and Technology

Integrating lasers with scanning tunneling microscopy (STM) allows the study of local photoexcitation and electron dynamics at the nanoscale. Implementing these techniques requires a reliable method to verify that modified STM tips can effectively collect localized photoelectrons. This study establishes setup within an ultra high vacuum (UHV) environment to validate this collection mechanism. We investigate the work function reduction of highly oriented pyrolytic graphite (HOPG) following the deposition of potassium (K) using an alkali metal dispenser. To measure the lowered work function, a continuous wave laser is modulated by an optical chopper, and the resulting photocurrent is measured through a biased amplifier setup. The photoemission threshold is determined by tracking the current as a function of sample bias. Auger electron spectroscopy (AES) is used to verify the presence and chemical purity of the deposited potassium, while low energy electron diffraction (LEED) characterizes the surface structure. By successfully measuring the photoelectric response of this low work function system, this work establishes the operational parameters and alignment protocols necessary for future experiments in conjunction with localized photoelectron collection in an STM.

Photoelectric Work Function Measurements of Potassium Doped HOPG

Richard Shulyak[1], Steven Poche[2], Dr. Jay Gupta[2]

[1] New Mexico Tech; [2] Ohio State University

Integrating lasers with scanning tunneling microscopy (STM) allows the study of local photoexcitation and electron dynamics at the nanoscale. Implementing these techniques requires a reliable method to verify that modified STM tips can effectively collect localized photoelectrons. This study establishes setup within an ultra high vacuum (UHV) environment to validate this collection mechanism. We investigate the work function reduction of highly oriented pyrolytic graphite (HOPG) following the deposition of potassium (K) using an alkali metal dispenser. To measure the lowered work function, a continuous wave laser is modulated by an optical chopper, and the resulting photocurrent is measured through a biased amplifier setup. The photoemission threshold is determined by tracking the current as a function of sample bias. Auger electron spectroscopy (AES) is used to verify the presence and chemical purity of the deposited potassium, while low energy electron diffraction (LEED) characterizes the surface structure. By successfully measuring the photoelectric response of this low work function system, this work establishes the operational parameters and alignment protocols necessary for future experiments in conjunction with localized photoelectron collection in an STM.

Tailoring the structure of amorphous grain boundary complexions in nanocrystalline copper alloys for enhanced plasticity

Esther Hessong[1], Timothy Rupert[2]

[1] Sandia National Laboratories; [2] Johns Hopkins University

Grain boundaries comprise a large volume fraction in nanocrystalline metals and are therefore microstructural features that are prime targets for engineering to meet a range of applications. Amorphous grain boundary complexions, a type of disordered grain boundary, are particularly promising due to their ability to act as efficient sinks for defects such as dislocations, which can lead to significant improvements in mechanical response, including both strength and plasticity. While grain boundaries can generally be classified as either ordered or disordered types, amorphous complexions can have different thicknesses and contain different levels of short-range structural ordering that can be tuned by planned doping and quenching treatments. To characterize amorphous complexions and their effects on mechanical behavior, electron microscopy and compression testing are employed in several different and advanced modes. First, amorphous complexions in Cu-Zr are used to improve bulk sample fabrication processing and subsequently demonstrate higher strength and plasticity. The amorphous complexions are studied in greater detail, specifically examining amorphous complexion thickness as a grain boundary descriptor and how this affects plastic failure mode. Further microcompression testing at elevated temperatures reveals that grains can coalesce and extrude at elevated temperatures, suggesting grain boundaries transition from ordered to disordered states at lower temperatures than previously thought for this alloy. Finally, increasing chemical complexity in ternary and quaternary Cu-rich alloys, dopant partitioning is quantified and correlated to changes in structural short-range ordering. In summary, by studying nanocrystalline Cu-rich alloys, we find that amorphous complexions are features that can be controlled through fabrication and processing steps to increase plasticity, addressing a major limitation of nanocrystalline materials.

Furan Maleimide Diels-Alder Chemistry Towards Self-Healing and Recyclable Products

Nusrat Yeasmin[1], Pabitra Choudhury[1]

[1] New Mexico Institute of Mining and Technology

In polymer science, furan and maleimides are widely used for Diels–Alder (DA) reactions, by which crosslinks are formed at moderate temperatures and de-crosslinking is achieved at higher temperatures via the retro-DA process. The dynamic covalent nature of these systems is considered promising for self healing, recyclable, and smart sustainable polymers. Mechanical strength is provided by stable networks at moderate temperatures, while rearrangement and recycling are enabled at elevated temperatures. DA efficiency is influenced by network strength and molecular design. Substituted furans and maleimides have been studied, with reaction rates calculated in various media using different basis sets. Reversibility depends on substituent effects. Recyclability is adversely affected by side reactions, with maleimide homopolymerization being the most common cause of irreversible crosslinking.

In this study, furan and various bismaleimides were used, and their reaction free energies, transition state barriers, and HOMO–LUMO energies were calculated. These calculations were performed to understand how different combinations alter reaction kinetics, material properties, recyclability, reversibility, and self healing behavior, while side reactions were controlled. Overall, furan–bismaleimide chemistry is regarded as a key strategy for designing functional polymers that satisfy both performance and environmental concerns.

Investigating (1-x)BiFeO3-xBaTiO3 as a Pb-free Ferroelectric Ceramic

Holden Chavez[1], Amanda Marotta[1], Tyra Douglas[1], Gabrielle Kamm[1], Eric Neuman[1], Daniel Lowry[1], Wen Dong[1], Mia Blea[1], Sean Bishop[1]

[1] Sandia National Laboratories

Currently, Pb(Zr/Ti)O3 (PZT) is the state-of-the-art ferroelectric ceramic due to its appealing electrical properties. However, the health and environmental hazards associated with lead-based materials have motivated the development of lead-free ferroelectric ceramics. One such alternative is (1-x)BiFeO3-xBaTiO3 (BF-xBT) because of its attractive piezoelectric properties coupled with high Curie temperature of ~475 °C (x = ~0.30). This research focuses on examining the electrical characteristics of BF-xBT for different x, with and without dopants. Additionally, the impact of processing parameters, including sintering conditions and controlled atmosphere annealing, on electrical properties are evaluated. These optimizations were made using a combination of electrical and structural characterization of the material, including the analysis of polarization-electric field hysteresis behavior, impedance spectroscopy, X-ray diffraction, and microstructural imaging.

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Proposed Investigation of Neutron or Gamma Radiation on the Mechanical Properties and Structure of GaN Semiconductors

Roberto Ruiz[1], Daniela Duarte[1], Dr. Brian Schuster[1]

[1] UTEP

This research introduces the synthesis and characterization of gallium nitride (GaN)-based oriented single crystals and nanocrystalline textured films utilizing Metal Organic Chemical Vapor Deposition (MOCVD). Previous work involved characterizing the resulting structures to evaluate their properties and identify localized disorder and defects. Additionally, preliminary probing of the nano-indentation response of synthesized GaN-based materials was done to estimate the distribution of critical resolved shear strengths. A proposed plan follows to irradiate GaN samples at varying dosage levels of neutron or gamma radiation and correlate the resulting changes in mechanical properties with respect to c- and m-plane orientations.

Preparation of Additive Manufactured Steel Surfaces for Nickel Electrodeposition

Alyssa A. DeLucia[1], Natalia Anna Saiz[1], Grace Shin[1], Veronica Gayoso[1], Joshua David Minster[1], Hannah Nicole Fowler[1], Benjamin White[1], Tylan Watkins[1]

[1] Sandia National Laboratories

Additive-manufactured (AM) stainless steels present higher surface roughness, porosity, and a thicker, non-uniform passive oxide layer relative to wrought alloys — surface states that undermine reliable nickel strike initiation and well-adhered electroplated films. Building on prior work, we incorporate electropolishing pretreatments to prepare AM 316 surfaces (powder-bed and bound-filament builds) for nickel strike and subsequent bulk nickel plating, with wrought 316 as a control. Length of electropolishing process and strike/plating workflows will be screened. Surface state will be quantified before and after pretreatment by optical profilometry and SEM. Film adhesion will be assessed by cross hatch test and quantitative solder-pin pull/bond tests; failure modes will be classified by SEM/EDX and cross-section imaging. Through this experimental framework, our goal is to develop general guidance and protocols that facilitate the achievement of well-adhered electroplated films on AM stainless steel surfaces.

Iron Sulfoselenide Catalysts for Bifunctional Oxygen Electrocatalysis in An-Air Batteries

Bryan Wygant[1], Jeremy Espano[1]

[1] Sandia National Laboratories

The growing need for grid-scale energy storage necessitates battery research and development. A promising candidate is the Zn-air battery, which is inexpensive, uses a non-flammable electrolyte, and can use abundant earth elements such as Fe and Mn. Zn-air battery development is limited by the performance of the Zn anode and the air cathode, the latter of which is the subject of this research. Here, we report the development of a family of iron sulfoselenide (FeSSe) bifunctional oxygen electrocatalyst (BOE) that can efficiently perform both the oxygen evolution reaction (OER) and the oxygen reduction reaction (ORR). This work builds on prior studies of nickel sulfoselenide (NiSSe) BOEs but seeks to replace costly Ni with abundant Fe. The use of inexpensive BOEs in Zn-air battery air cathodes would reduce the cost of battery development and deployment.

This work describes the synthesis and performance of the developed bifunctional catalyst (FeSSe) as a replacement for NiSSe materials. To create the mixed chalcogenide FeSSe compounds, we used a colloidal nanoparticle synthesis that allowed us to prepare particles with a single crystal structure (Fe_7X_8, X=S,Se) but a range of S/Se compositions. Techniques like X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDX) allowed us to confirm the preparation of FeSSe with S/Se ranging from 7:1 to 1:7.

After physiochemical characterization, material performance was evaluated through cyclic voltammetry (CV). Initial testing shows that S/Se composition does factor into catalytic performance, as it impacts the ORR, with Se-rich FeSSe showing better performance. Implementation of Ni into the FeSSe material shows improvements in OER but reductions in ORR, however, further study is needed for such quaternary systems. Ultimately, these results will be used to select the best performing FeSSe BOEs for testing in lab-scale Zn-air batteries.

This material is based upon work supported by the U.S. Department of Energy, Office of Electricity (OE), Energy Storage Division. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed herein do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Integration of an Acoustic Levitator into a SAXS/WAXS Instrument for Containerless X-Ray Scattering

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[1] Department of Aerospace Mechanical Engineering, The University of Texas at El Paso; [2] Department of Physics, The University of Texas at El Paso

Acoustic levitation is a great tool to facilitate the study of small solid or liquid samples, avoiding contact with sample holders. This provides little to no interaction with external components, therefore making it a container-less environment suitable for conducting X-ray scattering studies. X-ray scattering can be done in two settings: small-angle and wide-angle, each of them with their own characteristics. Small-angle scattering provides us a look into the nanometre structure of nanoparticles, pores, polymers, and droplets, whereas wide-angle scattering shows the atomic structure and crystallinity of materials, including crystal phases and molecular arrangement. This project focuses on adapting an acoustic levitator to operate inside a SAXS/WAXS instrument to enable in situ studies of droplets and solid samples under the confined conditions of the instrument. For this purpose, the best option was to use the TinyLev developed by the University of Bristol. This design was then adapted for the chamber of our SAXS/WAXS instrument by modeling and printing a mounting platform to achieve proper alignment and positioning along the path of the X-ray beam. Early SAXS experiments have been successful and demonstrated the feasibility of integrating both instruments to achieve containerless X-ray scattering data; because air causes interference in X-ray scattering data, current work focuses on developing a pressurized enclosure for the levitator to be able to operate under vacuum.

Wet Coating Nanosilica to Achieve High Limestone Content in Cement based Materials

Michael O'Donnell[1], Bu Wang[2]

[1] Department of Materials Science Engineering, UW-Madison; [2] Department of Civil Environmental Engineering, UW-Madison

Limestone can partially replace cement to reduce concrete carbon emissions, but higher replacement ratios reduce performance significantly. To achieve high cement replacement ratios while maintaining performance, we coated SiO2 nanoparticles, or nanosilica, onto the surface of limestone. Nanosilica has high pozzolanic reactivity and can compensate for the dilution effect of limestone. Traditionally, the main challenge of using nanosilica in cementitious materials is the tendency to agglomerate due to their high surface area, resulting in poor dispersion that limits their performance benefits. Coating them onto limestone resolves this issue.

In this study, we used a simple wet coating technique to fabricate nanosilica coated limestone, utilizing solution conditions that create opposite surface charges on nanosilica and limestone particles. We examine key parameters affecting the coating process, including solution conditions, silica to limestone ratio, and particle sizes. Cement paste samples containing the nanosilica coated limestone were benchmarked against control paste samples and samples containing the same materials but without coating. Results showed that nanosilica coated limestone improved mechanical properties and decreased pore volume. These results demonstrate that wet-coated limestone offers a promising strategy to achieve high cement-replacement levels while maintaining material performance.

Morphology-Aware Modeling of Photothermal Heating in TiN/Epoxy Nanocomposites

Leslie Elliot Ashie[1], Pabitra Choudhury[1], Sanchari Chowdhury[1]

[1] New Mexico Tech

Photothermal activation of thermoreversible polymers depends on both nanoscale optical absorption and composite-scale heat transport, yet these processes are often modeled independently. This study presents a morphology-aware electromagnetic thermal finite-element framework for clustered titanium nitride (TiN) nanoparticles embedded in an epoxy block. Frequency-domain simulations were conducted for close-packed clusters containing 1, 7, 19 ,37 and 61 TiN nanospheres with a diameter of 20 nm and an interparticle gap of 1 nm. Total and particle-normalized absorption were evaluated, and the position-resolved heat sources of the selected cluster were transferred into a periodic epoxy unit cell derived from the specimen geometry and a TiN loading of 0.5 wt.%. Transient heating was subsequently modeled under an incident irradiance of 12,500 W m^{-2}, with periodic lateral boundaries, convection at the exposed top surface, and an insulated bottom surface. Cluster-free epoxy blocks were added in the through-thickness direction to assess the influence of polymer volume and thermal mass. Although total absorption increased with cluster size, absorption per particle was highest for the 19-particle morphology. Central and edge particles within this cluster exhibited different absorption strengths because of their distinct electromagnetic environments. Nevertheless, rapid conduction over the short unit cell length scale produced a uniform temperature field. The one-, two-, and four-block configurations all approached approximately 146°C, which can exceed the retro-Diels–Alder activation range of 110–120 °C thus when the epoxy contains DA networks for selective for depolymerization. Increasing the amount of cluster-free epoxy progressively delayed the temperature rise but did not change the equilibrium temperature. This behavior follows the global energy balance: when absorbed power, convective area, and heat-transfer coefficient remain unchanged, added polymer increases the thermal time constant without altering the steady-state heat loss. The results distinguish the roles of nanoparticle morphology, source distribution, and polymer thickness: cluster morphology controls optical absorption, polymer thermal mass governs transient heating, and total absorbed power together with external boundary conditions determines the long-time temperature. The framework provides a transferable approach for designing photothermally activated polymer systems for repair, and reprocessing.

Design of Reusable Copper 101 Molds for Arc Casting

Samuel Jiron Tenorio[1], Brian E. Schuster[1]

[1] Dynamics Material Laboratory

Arc melting and casting technologies offer a versatile alternative to traditional casting techniques and procedures for novel alloys. These operations consist of using an electric arc to melt a metal charge, the molten metal is then transferred to a mold with an engineered cavity geometry. While there are existing molds provided by manufacturers and suppliers, end users may have different application needs that do not match the existing molds' philosophies. This study will detail the design phase and product verification of machined, reusable copper 101 molds that integrate a rectangular structure, a hemisphere, and an insert channel geometry. For the molds to be successful in casting operations, the design needs to ensure reliability, safety of operator and equipment, and perfect compatibility with the melter being used, all while withstanding vacuum conditions. Additionally, the design constraints and parameters behind the engineering decisions are discussed. The design of the mold will ensure compatibility with the Arcast Inc. ARC200 melter. The finalized products demonstrate that arc melting techniques are not limited to simple geometries or melter OEM molds. Finally, engineering recommendations are made for future mold designs and possible alternatives to final product design parameters.

Performance of Deep Eutectic Solvents as Electrolytes in Lithium ion Batteries

Martin Quintana[1]

[1] University of Texas at El Paso (UTEP)

Deep eutectic solvents (DESs) have emerged as promising alternative electrolytes for lithium-ion batteries due to their tunable physicochemical properties and potential for improved thermal stability. In this study, a betaine hydrochloride–citric acid (BeCl + CA) DES was investigated as an electrolyte for Ni-Co-Mn lithium-ion battery cathodes, with particular emphasis on how DES composition influences solid-electrolyte interphase (SEI) morphology. BeCl + CA DESs with molar ratios of 1:1, 1:2, 1:3, 1:4, 1:6, and 1:8 were initially evaluated for thermal stability at 65–70 °C, identifying compositions with increasing citric acid content that exhibited reduced stability and were subsequently excluded from further analysis. Scanning electron microscopy (SEM) coupled with computational image analysis was then used to characterize the resulting SEI morphologies, including surface roughness and average wrinkle spacing, as a function of DES composition. The remaining 1:1, 1:2, 1:3, and 1:4 compositions were further examined using wide-angle X-ray scattering (WAXS) to investigate changes in local structural organization associated with increasing citric acid concentration. These measurements were used to assess the evolution of solvation environments surrounding the DES components and to identify evidence of citric-acid-associated molecular networks that may develop at higher citric acid ratios. Together, the thermal stability, SEI morphological, and WAXS analyses provide a systematic framework for correlating BeCl + CA composition with interfacial structure and molecular organization, helping identify DES compositions with potential for stable and effective use as lithium-ion battery electrolytes.

Tailoring Silver Electroplated Films to Promote Uniform Lithium Cycling and Inhibit Dendrite Formation in Lithium Metal Batteries

Joshua Boyer[1], Tylan Watkins[1], Michael Urena[1], Melissa Meyerson[1], Leo Small[1]

[1] SNL

Lithium's high theoretical capacity (3860 mAh/g) and lowest reduction potential (-3.04 vs SHE) make it the prime candidate for high energy density battery anodes. However, researchers have long struggled to fully utilize Li anodes due to poor cycling behavior, namely, non-uniform electrodeposition and stripping from current collecting substrates and tendency to form dendrites. Both issues lead to low discharge/charge efficiency and dendrites can cause premature failure due to short-circuiting of the battery cell. Some research has shown that current collectors coated with lithiophilic metals (those fully miscible with Li) can lower the activation energy for Li nucleation—which promotes more uniform growth modes. Here, electroplated silver films on nickel substrates were investigated as lithiophilic promoters of uniform Li cycling. The study aimed to identify correlations between the structural properties of silver films and the cycling behavior of Li anodes.

This work was part of a Cooperative Research and Development Agreement (CRADA) with GridFlow, an energy storage company specializing in long-duration flow batteries.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Synthesis and Characterization of High Entropy, Low Thermal Expansion Oxides

Katherine Garcia[1], Tyra C. Douglas[1], Amanda S. Peretti[1], Sean R. Bishop[1]

[1] Sandia National Laboratories

Thermal expansion is a concern in applications with quick and substantial temperature changes, where resulting thermal shock can cause material failure. Materials that exhibit a negative thermal expansion coefficient (NCTE) are attractive to mitigate thermal shock as well as enable high precision technologies when used in combination with positive CTE materials to achieve an overall near zero CTE. High Entropy Oxides (HEOs) are a class of ceramic materials composed of several different cations, often added in equal concentrations, in a single phase that may offer unique advantages compared to conventional ceramics. For example, the high configurational entropy is believed to provide phase stability to the structure, and the presence of different cations may enable modifications to other properties besides CTE. In this presentation, the synthesis and characterization of an HEO with composition Zr0.4Mg0.4Al0.4Fe0.4Cr0.4Mo1.5W1.5O12 will be discussed, along with the challenges encountered in achieving a single-phase material.

Copper-Alumina Composite Coatings Via Kinetic Spray

Thomas Hands[1], Paul Fuierer[1]

[1] New Mexico Tech

Copper-alumina composite coatings can offer a desirable set of properties, combining the ductility and thermal conductivity of copper with the hardness of alumina, which may make them attractive for thermal management and surface protection. This research combines room temperature kinetic spray techniques to create unique, fine-grained particulate composites, and micro-laminates. Optimization of process parameters used for deposition of copper and alumina, both individually and combined, is necessary to obtain quality coatings. The microstructure and geometric properties are characterized using a combination of optical microscopy, scanning electron microscopy, x-ray diffraction, and optical profilometry. Preliminary physical properties, micro-hardness and apparent elasticity via indentation, and thermal conductivity via transient plane source measurements, will be presented.

Strength and Failure Modes of Ceramic and Composite Dielectric Films Made by Dry Aerosol Deposition

Nigel Horak[1], Paul Fuierer[1]

[1] New Mexico Institute of Mining Technology

Dry aerosol deposition (DAD) produces dense ceramic films at room temperature by high kinetic energy spraying of dry powder onto a substrate, where particles fracture and bond on impact. This work maps the mechanical reliability of barium neodymium titanate (BNT) films and BNT-polymer composites on copper, glass, and a circuit-board laminate (FR2). Films were sprayed in a fixed process window. Tensile pull-off testing was paired with fracture-surface inspection to tell whether failure started in the testing adhesive, at the film-substrate interface, or inside the coating. Thicker coatings (on FR2) allow complimentary analysis using X-ray micro-computed tomography (mXCT) so buried defects can be compared with coating failures. Diffraction and electron microscopy check whether grain size and morphology change as the coating builds.

Thickness was the main control. Thin, dense films were often stronger than the adhesive used to test them. As coatings grew thicker, strength fell and failure moved into the film, consistent with more internal defects and stored residual stress. A smoother copper finish produced higher strength than a coarse finish. At moderate thickness, copper, glass, and FR2 performed similarly. A post-deposition anneal did not change peak strength in a systematic way. Polymer additions did: PTFE blends formed thick but poorly bonded coatings that failed internally, and even a small polyimide addition reduced strength and made continuous growth harder.

Data-Driven Methods for Predicting Electrochemical Migration in Electronic Components

Janice Yeung[1], Jarod Kaltenbaugh[2], Matthew Kottwitz[2], J. Elliott Fowler[2], Kristopher O. Davis[2]

[1] Graduate intern (sandia national laboratory-New Mexico); graduate researcher (university of central Florida), [2]Sandia National Laboratories

No-clean solder fluxes are used in electronics manufacturing because they eliminate the need for a post-soldering cleaning step, but residues left behind can absorb moisture and become ionically conductive, creating conditions favorable for electrochemical migration (ECM). ECM is a major cause of degradation and failure in electronic components. In humid environments under electrical bias, ion transport can lead to dendritic shorting and device failure. Characterization has relied on time-intensive manual testing and visual inspection, limiting the scale and consistency of data available to study degradation.

This work advances the characterization of ECM in electronic components using interdigitated comb (IDC) sensors through a custom-built, open-source, Python-based automated testing platform. The IDC sensors used in this research are capacitive structures with varying finger geometries and spacing, printed on FR-4 substrates using copper or ENEPIG traces. A subset of boards feature solder masks.

Custom 3D-printed wells are attached to individual sensors, isolating each sensor from its neighbors, and each is flooded with weak organic acids or deionized water to simulate no-clean flux residue contamination, with electrical bias applied at 3 or 5 volts to accelerate dendritic growth. The system integrates multimodal data collection of electrical measurements and imaging with automated hardware control, logging parameter changes alongside time-stamped, correlated metadata. This closed-loop automation enables high-throughput, consistently-labeled dataset generation without continuous manual operation.

Preliminary testing has been completed on a series of IDC sensors, validating the platform's data collection and logging pipeline. Using a 12MP camera capturing time-series imaging, dendritic growth was visually detected and time-to-failure was recorded to the second. Testing of an additional 400 sensors is planned to build a dataset of the scale needed for robust degradation modeling.
Reliable prediction of ECM is critical for electronics used in humid, high-reliability, or field-deployed environments, where undetected degradation can lead to costly failures. The next step for this operational infrastructure is incorporating artificial intelligence and machine learning approaches to correlate imaging and electrical signatures with ECM progression, for predicting time-to-failure and identifying degradation indicators before permanent failure occurs.

Design and Thermal Analysis of a Heated Mold for Improved Infiltration of 316L Stainless Steel–A356 Aluminum Composites

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Composites have been utilized in numerous industries that require a high strength-to-weight ratio; however, the development of composites has been limited by the complexity of processing and material compatibility. Recent interest in composite research has led to the reliable manufacturing of metal-metal matrix composites, such as 316L stainless steel matrix composite reinforced with A356 aluminum in a gyroidal configuration. To improve the manufacturing of this composite, heated molds have been designed to improve infiltration by using cartridge heaters to maintain a controlled temperature between 300℃ - 500℃ in a stable inert environment. Simulation software such as ANSYS has allowed us to map out the heat transfer and model the heating process to evaluate the effectiveness of the cartridge heater placement and overall performance of the design. During casting, thermocouples will be incorporated into the mold to measure the temperature at selected locations. The thermocouple measurements will provide feedback to regulate the power supplied by the cartridge heaters to maintain the desired temperature. Thus, by combining heat transfer simulations, experimental measurements, and a temperature control system, this experimentation aims to develop a reliable, heated mold that improves the infiltration of A356 aluminum into the 316L stainless steel gyroid, producing a more consistent, high-quality composite.

Determination of the Dielectric Permittivity of DAD Dense Lunar Dust Using IDE Architecture

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Future lunar missions emphasize the fabrication of materials and components, including electronic, on the Moon using available in-situ resources (ISRU). This work considers building electronic films and components from lunar dust (simulant) using Dry Aerosol Deposition (DAD), which is a novel additive manufacturing process using only kinetic energy for densification, and is highly suited for the moon's dry and vacuum environment. Thick, dense dielectric ceramics may provide both shielding from the extremes and serve as functional dielectric layers of passive electronic components. Designing capacitive devices for sensing, energy storage, gas monitoring, water-ice detection, and electrostatic control coating requires knowledge of the dielectric properties of the regolith. This study involves the deposition of lunar dust onto interdigitated electrode (IDE) structures and develops a precise and accurate method for determining the relative permittivity (εr) of fully dense, nano-structured mineral ceramic via combination of capacitance measurement and COMSOL simulation. Experiments reveal densified lunar highlands simulant (LHS-1D) to have permittivity in the range ~2.98 to 3.92 over temperature range of -20 °C to 100 °C. Lunar mare, with more diversified mineral content, including ilmenite and olivine, has higher permittivity of ~6.89 to 8.27. Results are discussed in the context of deposition quality, dielectric polarization mechanisms, simulation parameters and measurement error. Preliminary attempts at building a complete IDE device using DAD will be shown.

Keystone Semantic Catalog: A Layer for Materials Data Discovery

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Materials characterization data is oftentimes difficult to discover and reuse as the same scientific concepts or ideas appear under many different names across instruments, workflows, and datasets. In Keystone, a governed data lakehouse for materials data, current infrastructure includes where the data is stored and who can access it, but not necessarily what the data means. This project investigates the effectiveness of a lightweight semantic layer for Keystone that improves data discovery and supports AI-assisted retrieval.

The prototype semantic layer organizes metadata into a five-table semantic schema with concepts derived from existing Pydantic data models. The layer captures cross-dataset terminology, such as alternate field names, abbreviations, measurement relationships, and test-family hierarchies, while preserving the distinction between semantic meaning and governed data access.

To explore question-driven data discovery, a Python-based prototype was developed to resolve natural-language phrases into canonical concepts, expand related concepts, and identify relevant tables and columns. The design supports exact phrase matching, typo handling, and future semantic retrieval workflows with automatic semantic layer mapping for future datasets.

Process Development of Low Temperature ALD of Bismuth Oxide using Novel Precursor

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Bismuth oxide (Bi2O3) is a functional oxide that exists in five crystalline phases and has applications in optics, sensors, microelectronics, and photocatalysis. Bi2O3 thin films that are grown by chemical vapor deposition (CVD) or atomic layer deposition (ALD) often require higher temperatures to drive surface chemistry which can cause non-stoichiometric, oxygen deficient films.

Herein, we develop a novel thermal ALD process using methyldiphenylbismuth (MePh2Bi) and ozone. MePh2Bi is more volatile and thermally stable than other precursors, such as triphenylbismuth (Ph3Bi). This results in crystalline (δ-phase), stoichiometric films and allows for lower deposition temperatures, enabling deposition on thermally sensitive substrates. We observed precursor saturation at temperatures as low as 90 °C, with a growth per cycle (GPC) of 0.6 Å/cycle within the ALD window of 100-170 °C. The films were characterized by X-ray photoelectron spectroscopy (XPS), spectroscopic ellipsometry (SE), atomic force microscopy (AFM), and grazing incidence X-ray diffraction (GIXRD).

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Parameters Required to Encourage Phase Changes and Self Pulverization in the Extraction of Alumina from Coal Clinkers

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Alumina (Al2O3) was extracted from for a vein of clinkers from the San Juan Basin of New Mexico using the lime sinter method. One difficulty that needs to be taken into account when using the lime-sinter process is achieving consistent self-pulverization of the post sintered material. It was discovered that the self-pulverization is highly dependent on two factors: the molar volume expansion of larnite (Ca2SiO4) when transforming to a calcio-olivine polymorph, and the decrease in molar volume during dissociation of mayenite ((CaO)12 · (Al2O3)7) into several phases. To encourage the larnite/olivine transition and the mayenite breakdown of the sintered material, several process parameters need to be implemented. These parameters are slow cooling from the maximum temperature of 1360oC, a high in silica content and low in moisture in the raw ore, and an oxidative atmosphere. This resulted in a fine, leachable powder that could then be processed to form alumina.

Correlating Chemistry and Microstructure in Advanced Materials via AFM-IR (NanoIR)

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The ability to simultaneously map chemical identity and physical topography at micro- and nanoscale is essential for the development and failure analysis of advanced materials. Nanoscale infrared spectroscopy (NanoIR) achieves this by integrating atomic force microscopy (AFM) with localized IR excitation, bypassing the diffraction limit of traditional IR spectroscopy to provide chemical mapping at the nanoscale.

I will present the application of NanoIR across a diverse suite of materials to demonstrate its versatility as a characterization platform. I will discuss its application in structural polymers and composites, specifically focusing on the assessment of interfacial continuity in laminates and the phase morphology of epoxy blends. Furthermore, I will present the tool's efficacy in root-cause failure analysis, demonstrating the localization and identification of trace polymeric residues and contaminants on electronic components. To illustrate the broader reach of the technique, I will briefly touch upon its application in characterizing the microstructure of additively manufactured metal alloys and bio-aerosols.

By providing a direct correlation between chemical "fingerprints" and nanoscale structure, NanoIR serves as a critical tool for materials scientists working on everything from sustainable polymers to advanced manufacturing. This presentation will highlight the capabilities, limitations, and practical workflows required to implement NanoIR in a materials characterization pipeline.

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Next-Generation Paper-Based Uric Acid Sensor Enabled by Nickel–Indium Sulfide Nanostructures

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Uric acid is an important biomarker in urine, and elevated levels are associated with conditions such as gout and kidney dysfunction. Therefore, the development of low-cost, sensitive, and portable detection methods is essential for point-of-care monitoring. In this study, we present a nickel indium sulfide (Ni–In–S) nanomaterial–modified paper-based electrochemical sensor for the rapid detection of uric acid. The sensor was fabricated by drop-casting trace amounts of Ni–In–S nanomaterials onto the working electrode of a paper-based platform, which enhances electrochemical performance by increasing surface area and improving electron transfer efficiency. The modified sensor exhibits improved sensitivity and a lower limit of detection compared to the unmodified paper electrode, demonstrating its effectiveness for uric acid sensing. Overall, this work highlights the potential of Ni–In–S modified paper-based sensors as a simple, cost-effective, and portable platform for on-site biomarker detection and point-of-care diagnostics.

CO_2 Binding on K_2O: Effects of Cluster Size and Surface Facets

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Rising atmospheric CO_2 levels have increased the need for efficient carbon capture materials. Alkali metal oxides such as K_2O are promising because of their surface basicity and low cost, but strong CO_2 binding to bulk K_2O can make desorption energy-intensive. This study used DFT calculations to investigate CO_2 adsorption on bulk K_2O and clusters of different sizes, showing that smaller clusters bind CO_2 more weakly than larger clusters and bulk surfaces. Experimental TGA and DSC results supported this trend. The study also found that supporting K_2O clusters on γ-alumina significantly strengthens CO_2 binding, demonstrating that both cluster size and support material strongly influence CO_2 adsorption.

Rapid Electrochemical Biomarker Detection Using Laser-induced Graphene Sensors

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Laser-induced graphene (LIG) has become a promising material for electrochemical biosensors because of its excellent electrical conductivity, large surface area, porous three-dimensional structure, and simple fabrication process. The project investigates the use of LIG to develop low-cost, rapid diagnostic test strips for detecting key biomarkers such as dopamine, uric acid, and ascorbic acid. The unique electrochemical properties of LIG enable sensitive and selective detection of very low biomarker concentrations, making it a strong candidate for point-of-care diagnostic applications. In addition, LIG can be produced using a single-step laser scribing process under normal environmental conditions, eliminating the need for complicated synthesis techniques and helping lower production costs. The ability to adjust laser power and scanning parameters also enables the creation of reliable, reproducible sensing platforms at scale.

Another advantage of LIG-based sensors is the ability to integrate biomolecule-specific recognition elements onto the electrode surface, which improves sensor selectivity and overall analytical performance. This allows for more accurate detection of biomarkers in complex biological samples. Because of these benefits, LIG-based biosensors have the potential to serve as practical and accessible healthcare diagnostic tools, especially in rural and underserved areas. This technology is particularly relevant to the Navajo Nation, where long travel distances and limited access to specialized healthcare services can delay diagnosis and treatment. By providing a rapid, affordable, and portable method for monitoring biomarkers, LIG-based sensing platforms could support earlier disease detection, improve personalized healthcare, and contribute to better health outcomes in indigenous and other resource-limited communities.

Real-Time Spatial Mapping of Heavy Metal Contamination Using a 3D-Printed Electrochemical Sensor Boat

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Heavy metal contamination in natural waters remains a significant environmental and public health concern, particularly in regions affected by legacy mining activities and mineral-rich geologic formations. Traditional laboratory-based water quality assessments provide only discrete measurements from individual sampling locations, limiting the ability to characterize the spatial distribution of contaminants across entire water bodies. Here, we present a fully 3D-printed autonomous electrochemical sensing boat that integrates thread-based ion-selective electrodes (ISEs) with square-wave anodic stripping voltammetry (SWASV) for the real-time detection and quantification of Pb^{2+}, Cu^{2+}, and Cd^{2+} in natural waters. The thread-based ISEs function as a preliminary screening system, triggering SWASV analysis only when elevated metal concentrations are detected, thereby reducing reagent consumption, electrode fouling, and power requirements while maintaining high analytical sensitivity. An onboard ESP32 microcontroller processes electrochemical signals, converts them into calibrated concentration values, and wirelessly transmits the data to a web-based user interface.

Each measurement is linked with GPS coordinates, enabling the automatic generation of real-time concentration profiles and high-resolution contamination maps. Unlike conventional water testing approaches that identify contamination only at isolated sampling points, this platform provides comprehensive spatial information revealing contaminant distribution patterns, pollution hotspots, and potential transport pathways. The platform is especially relevant for monitoring water resources in and around the Navajo Nation, where concerns regarding heavy metal contamination from historical mining operations and natural mineral deposits continue to impact environmental and community health. By combining low-cost electrochemical sensing, autonomous operation, onboard data processing, GPS-enabled mapping, and real-time visualization, this technology offers a scalable and accessible tool for identifying contamination sources, supporting remediation efforts, and improving water quality monitoring in rural and underserved communities.

Stoichiometric Differences in Phase Stability of Ion Irradiated Yttrium Hydride and its Relation to Microreactor Applications

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Due to the extreme environments of advanced nuclear reactors, such as microreactors, new materials are being investigated that can withstand these conditions. One such material is yttrium hydride, but its response to irradiation, especially under high temperatures, must be further investigated. For this purpose, 9 samples were fabricated at Los Alamos National Laboratory, with H/Y ratios of 1.6, 1.8, and 2. For each stoichiometry, one sample was left as-fabricated, one was subjected to a 400°C environment, and one was irradiated with 9MeV Au3+ ions at 400°C at the University of Tennessee, Knoxville. Through Raman spectroscopy, grazing incidence x-ray diffraction, nanoindentation, and transmission electron microscopy, the effect of both high temperature and ion irradiation on hydrogen retention was analyzed. From this characterization, it was found that rapid hydrogen loss was observed in YH1.6 and YH2 samples regardless of irradiation, but hydrogen retention increased in YH1.8 with ion irradiation. Through these characterization techniques and tailored ion beam irradiation, the use of yttrium hydride as a moderator for microreactors can be better understood, and its limitations can be determined.

Design of an achromatic Phase Fresnel Lens for 3D printing via 2 photon polymerization

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Focusing X-rays is fundamentally different from focusing visible light in that X-rays pass through almost all materials with almost no bending, making them difficult to refract. High-resolution X-ray imaging can instead be built on diffractive optics such as Phase Fresnel Lenses (PFLs), which are a repeated pattern of continuous sawtooth shaped profiles spaced at a multiple of the design wavelength. To overcome the inherent wavelength specificity and resulting chromatic aberration, we turn to achromats, which tune the focus across a broader energy band. Previous achromats have been standalone structures requiring alignment to the lens, or multi-process structures fabricated on a single substrate. In response, we aim to create a monolithic X-ray PFL optic with an integrated achromatic profile. However, producing a smoothly graded, high-aspect ratio 3D profile at sub-micron zone widths is challenging for lithography and chemical etching. Two-photon polymerization direct-write printing offers another approach, by enabling structures to be built voxel by voxel with grayscale control over exposure dose, it can natively produce the phase ramps a PFL requires without the multi-step processing needed to approximate one lithographically. This lens was designed for space-based imaging of compact, high-energy astronomical sources (such as black holes, neutron stars, pulsars, and X-ray binaries) which all benefit from a narrow field of view and very high angular resolution. It is simultaneously designed for fabrication via 2PP printing, ahead of a proposed fabrication and test campaign.

Formation of fluorinated passivation layers on aluminum current collectors for corrosion protection in battery electrolytes

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Current collectors are important battery components that provide the conductive pathway for electrons from the electrode active material to the external circuit. Despite not participating in the energy storage reactions, the current collectors can significantly impact overall lithium-ion battery performance. Current collectors are typically made from thin (~10-20 μm) Al foil for the cathode and Cu foil for the anode. Degradation of current collectors is typically via corrosion, which results in the dissolution of metal. Metal ions from metal dissolution can be redeposited elsewhere in the battery and contribute to crosstalk phenomena. Current collector corrosion can lead to poor contact at the current collector/active material interface and detrimental changes to electrolyte composition. This work focuses on benchmarking corrosion behavior and mechanisms of the cathode's Al current collector, because the current collector experiences a particularly strong oxidizing environment in high voltage (>4.2 V vs Li/Li+), next-generation lithium-ion batteries. The corrosion stability of the Al current collector is strongly influenced by the electrolyte composition: lithium hexafluorophosphate–based electrolytes can passivate the Al surface up to ~5 V by fluorinating the native aluminum oxide. Conversely, corrosion occurs readily at <5 V in lithium bis(fluorosulfonyl)imide- and lithium bis(trifluoromethanesulfonyl)imide-based electrolytes. This work identifies corrosion trends on Al current collectors as a function of electrolyte composition and surface chemistry. Mechanistic explanations of observed trends are also presented.

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High-Rate Compression Characterization of Polyurethane Foams Using Split Hopkinson Pressure Bar Methods

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Polyurethane foams are widely used as energy-absorbing materials in Sandia weapons systems due to their favorable deformation characteristics. This study experimentally investigates the compressive behavior of commercial and stockpile polyurethane foams across a broad range of material densities, from 5 pcf to 40 pcf, and strain rates, from 10-3 s-1 to 104 s-1. Both confined and unconfined experiments were conducted on several test frames. These frames included a 100 kip MTS servo hydraulic test frame, a Bionix servo hydraulic test frame, and a Split Hopkinson Pressure Bar (SHPB) to fully span the strain rate regime, and ensure adequate force measurement resolution. This presentation highlights the experimental techniques used to refine the SHPB tests, and the steps of data processing. Experimental parameters such as bar material, applied pressure level, signal conditioner settings, and striker bar length were optimized for foam density. Less dense foams required using polycarbonate bars and lower pressure, while more dense foams required the maraging steel bars and higher pressures. A MATLAB-based script was developing for processing the voltage signals from the strain gages on the incident and transmission bar. The code converted these signals into specimen stress-strain response using one-dimensional wave theory. This presentation details the refined experimental SHPB testing methodology, data processing techniques, and key findings on the rate-dependent compression behavior of polyurethane foams. These test provide insight relevant to their application in energy absorption and future testing.

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