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Oral Presentation & Poster Program Abstracts

Symposium Chair: Elliott Fowler

Symposium Co-Chair: Jessica Buckner

Oral Presentation Abstracts

AutoSciLab: A Self-Driving Laboratory for Interpretable Scientific Discovery

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Speaker: Saaketh Desai

****INIVTED PRESENTATION****

Advances in robotic control and sensing have propelled the rise of automated scientific laboratories capable of high-throughput experiments. However, automated scientific laboratories are currently limited by human intuition in their ability to efficiently design and interpret experiments in high-dimensional spaces, throttling scientific discovery. We present AutoSciLab, a machine learning framework for driving autonomous scientific experiments, forming a surrogate researcher purposed for scientific discovery in high-dimensional spaces. AutoSciLab autonomously follows the scientific method in four steps: (i) generating high-dimensional experiments using a variational autoencoder (ii) selecting optimal experiments by forming hypotheses using active learning (iii) distilling the experimental results to discover relevant low-dimensional latent variables with a 'directional autoencoder' and (iv) learning a human interpretable equation connecting the discovered latent variables with a quantity of interest ($y = f(z)$), using a neural network equation learner.

We validate the generalizability of AutoSciLab by rediscovering a) the principles of projectile motion and b) the phase-transitions within the spin-states of the Ising model (NP-hard problem). Applying our framework to an open-ended nanophotonics problem, AutoSciLab discovers a new way to steer incoherent light emission beyond current state-of-the-art, defining a new structure(material)-property(light-emission) relationship governing the physical process using closed-loop noisy experimental feedback.

Discovery of Conductive Nanoparticle Inks for Printed Electronics using an Autonomous Ecosystem

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Speaker: Allie Roth

Conductive nanoparticle inks (i.e. Cu, Ag, Au) are critical technologies for additively manufactured electronics, but they often suffer from reduced conductivity and robustness under stress. We believe that integrating artificial intelligence and machine learning with autonomous synthesis processes will significantly expedite ink discovery and optimization for next generation printed electronics. To this end, we are developing an autonomous ecosystem to selectively target and characterize monodisperse silver nanoparticles using high-throughput methods. Our central hypothesis is that the nanoparticle properties, ink printing processes, and resulting conductivity can be optimized by manipulating the stoichiometric ratio of nanoparticle surface functionalizing ligands as well as the concentration and chemical composition of reducing agents. Utilizing a custom Bayesian optimization algorithm to assess the nanoparticle properties and inform our new design of experiments, we demonstrate an iterative process for rapidly optimizing synthetic parameters that will accelerate synthesis and fabrication strategies for metal nanoparticle inks.

Impact of Thermal Gradient on Interfacial Energy and its Anisotropy in Al-Cu Alloy

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Speaker: Amrutdyuti Swamy

Additive manufacturing (AM) has transformed production by enabling the creation of intricate geometries, reducing material waste, and facilitating the customization of parts. Despite these advantages, the application of AM to metals, particularly Al-Cu alloys, is challenged by the formation of microscopic defects, such as cracks and porosity, during solidification. A promising approach to reduce these defects is by increasing the fraction of equiaxed grains in the microstructure. This study explores methods to enhance equiaxed grain formation in Al-Cu alloys during rapid solidification using molecular dynamics simulations. We investigate the solid-liquid interface of an Al-Cu system under varying Cu concentrations and thermal gradients. Building on prior research that demonstrated the promotion of oriented equiaxed grain formation with Cu content above 8.8 at. %, we introduce a thermal gradient across the solid-liquid boundary to replicate realistic rapid solidification scenarios. We evaluate the combined effects of Cu concentration and thermal gradient on microstructural evolution and analyze the changes in interfacial free energy and anisotropy in response to the applied thermal gradient.

Robust Data-Driven Run-to-Run Control for Automated Serial Sectioning

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Speaker: Rhianna M. Oakley

Automated mechanical serial sectioning (MSS) is an advanced characterization technique that provides detailed microstructural information across large length scales. By repeatedly removing thin layers of material and imaging the exposed surfaces, MSS constructs a 3D representation of a sample's internal structure, enabling failure analysis and feature identification in samples that are otherwise inaccessible via conventional 2D or non-destructive evaluation techniques. However, achieving consistent and precise material removal in MSS is challenging due to inherent variability and disturbances in mechanical grinding operations. Typically, an experienced operator must manually select MSS parameters to achieve the desired material removal thickness, prolonging data collection times and necessitating post-processing routines to standardize the data.

A robust approach to ensure reliable performance and accurate microstructural characterization, especially for multi-material compositions was employed to address these challenges. We present a one-step model predictive control (MPC) framework tailored to a run-to-run (R2R) controller. The R2R-MPC controller automates the MSS process, improving the consistency of material removal. Embedded in an R2R framework, the controller provides iterative feedback for disturbance rejection and convergence to the desired removal rate. Without an analytic model of the MSS system, we employ a data-driven approach to synthesize the controller, ensuring adaptability to specific material characteristics. The effectiveness of the R2R-MPC controller is demonstrated through simulations and experimental results with a real MSS system. This automated approach significantly enhances the accuracy and reliability of microstructural data, facilitating applications in reverse engineering and failure analysis.

Full-Field Micromechanical Modeling of 3D Polycrystals with Recurrent Neural Networks

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Speaker: Ashley Lenau

High energy diffraction microscopy (HEDM) is a non-destructive characterization technique that studies a material's evolution during a mechanical load. As valuable as HEDM is, the extensive planning, data collection and time needed for a successful experiment can make it an expensive endeavor. Numerically based crystal plasticity simulations may allow for better experimental planning but are still too slow to be used in real time with an experiment. Deep learning models are fast enough for real time feedback that could focus data collection and could increase the design space for experimental planning. However, deep learning is currently limited by the small training datasets available. This work proposes a U-Net model with recurrent connections to predict the full-field micromechanical evolution of a 3D Cu polycrystal and investigates the transferability of this network on three different material datasets. The possibility of using the Cu-trained network as a building block to incorporate additional materials into the model's capability is explored.

Computationally-efficient DFT calculations for elastic properties of refractory binary alloys

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Speaker: Surya Bijjala

The elastic constant tensor (ECT) is an important property that describes alloy behavior under external stresses within the elastic limit. It thus provides insights into the effects of strain on the mechanical properties of materials. ECT can guide the design of new refractory alloys/refractory high entropy alloys with improved mechanical properties. Here, we report computed elastic properties for structural BCC binary alloys of Mo, Nb, Ta, and W, elements of the structural refractory family, using first-principles-based density functional theory (DFT) calculations as implemented within the ABINIT electronic structure code. The rigid ion elastic tensor was computed using density functional perturbation theory with strain perturbation, followed by atomic relaxations to yield the relaxed ion elastic tensor. This approach has been shown to be significantly more efficient than the traditional stress-strain method, thus opening a path to high-throughput calculations for these materials. The results of both rigid ion ECT alone, and relaxed ion ECT for the BCC solid solutions of the binaries are in excellent agreement with available experimental data and other first-principles results. Derived polycrystalline aggregate properties—bulk modulus (B), shear modulus (G), Young's modulus (E), elastic anisotropy, and Poisson ratio (v)—are reported. The computed data establishes a foundation for the systematic design of high-temperature structural refractory alloys with desired mechanical properties.

Atomic Precision Advanced-Manufactured (APAM) FET-based sensor for ultrasensitive charge sensing

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Speaker: Juan Mendez

Recently, Atomic Precision Advanced Manufacturing (APAM) technology has enabled the creation of 2D doped structures (also known as δ-layers) in semiconductors with single-atom precision and very high dopant densities, much higher than the solid solubility limit. APAM is a process to incorporate dopants, such as P or B, at the atomic scale into Si surface using chemistry surface. APAM has various applications, including the exploration of novel nano-scale electronic devices for classical computing, quantum computing and quantum sensing.

In this work, we explore the use of APAM δ-layer tunnel junctions as ultra-sensitive devices for charge sensing in a broad spectrum of applications, such as biological, chemical, radiation and nuclear detection. The proposed device consists of two highly-conductive P δ-layers separated by an intrinsic gap embedded in Si (Si: P δ-layer tunnel junction). To carry out this study, we employ our quantum transport framework, based on the Non-equilibrium Green Function (NEGF) and the effective mass theory. We have found that these devices can easily detect single charges near the junction by observing measurable changes in the electrical current. Our simulations show that the tunneling current between δ-layers is strongly affected when the charge is present in the proximity of the tunnel junction: the current increases by the presence of negative charges, whereas decreases by the presence of positive charges. We also demonstrate theoretically that these devices exhibit superior sensitivity than convectional FET and tunnel FET-based sensors in the low-charge concentration limit. Our simulations demonstrate that our APAM FET-based sensor achieves a sensitivity of S=0.95 at 300K and a sensitivity of S=7 at 4K, compared to a theoretical sensitivity of S=6e-3 for tunnel FETs-based sensors. In addition, we postulate that the extreme sensitivity of δ-layer tunnel junctions to the presence of charges arises from the strong quantization of the conduction band in these highly-confined systems, which is the result of the confinement of the dopants in one direction. In addition to their extreme sensitivity to the presence of charges, these devices also offer significant advantages such as i) they are exceptionally simple two-terminal devices; ii) they are extremely small-size, of the order of 10 nm; and iii) suitable for integration with CMOS technology.

Nickel-Based Single-Atom Catalyst for Methane Pyrolysis

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[1]NMT Chemical Engineering

Speaker: Naomi Helsel

Sustainable hydrogen production from natural gas with the added advantage of permanent carbon capture has sparked renewed interest in methane pyrolysis. Development of suitable catalytic systems for methane pyrolysis requires a detailed investigation of the C−H bond activation energies on those catalysts as well as their stability against sintering and coke formation. Using ab initio spin-polarized density functional theory (DFT) calculations, both the single-metal Ni atoms and small clusters of Ni atoms deposited on titanium nitride plasmonic nanoparticles have been investigated for methane pyrolysis. Combined computational and experimental results suggest that single Ni atoms can favorably be deposited on N-vacancy sites on the TiN surface. Complete reaction methane pyrolysis pathways, including the C-H bond-breaking transition steps and CHx fragments, were studied in the present work for the Ni systems. The activation energy barriers were facile for both systems with the Ni clusters having a lower barrier than the single atoms. The single atom system showed weaker adsorbate binding and a net endothermic reaction pathway to suggest that it can resist surface coke formation. However, the single atoms are suspected to sinter, aggregate into small clusters, and then form a coke layer due to the highly exothermic pathway of the cluster despite its high activity.

Focused Ion Beam Low Energy Implantation

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Speaker: Alex Belianinov

****INVITED SPEAKER****

Ion implantation is a key capability for the semiconductor industry. As devices shrink, novel materials enter the manufacturing line, and quantum technologies transition to being more mainstream, traditional implantation methods fall short in terms of energy, ion species, and positional precision. However, lowering the implantation energy while maintaining nanometer scale spot size is a technological challenge. This presentation will show an overview of techniques at Sandia National Laboratories Ion Beam Facility that allow focused ion implants 10-200 keV range for quantum relevant applications. Additionally new developments in sub-1 keV focused ion implants into Si and 2D devices, using a focused ion beam system, validated by atom probe tomography will be shown. We illustrate that identical results for low energy ion implants can be achieved by either lowering the column voltage, or decelerating ions using bias – while maintaining good spatial resolution. Furthermore, our data reveal that standard implant modeling approaches overestimates experimental depth by a significant margin. Finally, we discuss how our results pave a way to much lower implantation energies, while maintaining high spatial resolution.

Optical Response of MXene Nanoantennas Under Left and Right Circularly Polarized Illumination

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Speaker: Vahid Karimi

The exploration of optical chirality in nanoantenna arrays has significant implications for advanced optical communication, sensing, and imaging. Optical chirality, a property where a structure exhibits different interactions with left-handed and right-handed circularly polarized light, is crucial for developing novel technologies in these fields. This study investigates the chiral properties of nanoantenna arrays designed from highly absorbing MXene materials, which are known for their distinctive electronic and optical characteristics.

Leveraging the unique lattice resonances arising from the periodic arrangement of MXene nanoantennas, we demonstrate enhanced chiral responses in the visible and near-infrared spectral ranges. The periodic arrangement of these nanoantennas creates specific resonant modes that amplify chiral interactions, thereby improving the overall chiral response. The intrinsic lossiness of MXene, often considered a limitation due to its absorption properties, is mitigated through the lattice design. This approach facilitates the achievement of stronger resonances and improved light–matter interaction, effectively countering the material's lossiness.

We compare the optical responses of various MXene compositions, including titanium carbide (Ti_3C_2), titanium nitride (Ti_3N_2), and its oxidized form ($Ti_3N_2O_2$). By evaluating these different materials, we show how the composition influences chiral optical properties, contributing to a deeper understanding of how material characteristics impact chiral behavior. Our findings highlight the potential of chiral MXene metasurfaces for applications in biosensing and polarization-sensitive photodetection. These applications are critical for developing advanced photonic devices that can offer enhanced performance and new functionalities in various technological domains.

References:

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Probing Charge Trapping of High k Dielectric Stacks under Ionizing Radiation

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Speaker: Devika Mehta

The integration of high k dielectrics in metal-oxide-semiconductor (MOS) devices has been revolutionary for advancing conventional semiconductor devices due to their low leakage and thermal stability at exceedingly low effective oxide thicknesses. Under ionizing radiation, electron-hole pairs are generated in the dielectric stack and subsequently trapped, in the form of oxide trapped charge or as interface traps, creating a charge buildup that results in a measurable shift in the flatband or threshold voltage of a MOS capacitor or MOS field effect transistor (MOSFET), respectively. Here, we evaluate and report the response of multilayer dielectric stacks to x-ray exposure, with a focus on observing charge trapping through the layers, in an effort to understand the behavior of these materials and their interfaces for integration in electronic devices.

Dielectric films of HfO2 and Al2O3 are successively grown via atomic layer deposition (ALD) and fabricated into MOS capacitors on a p-type Si substrate with an aluminum top gate. The thicknesses and layering of the dielectric layers were selected to assess how charge is generated, tunnels and recombines. Charge can be trapped via a mismatch in mobility between holes and electrons as well as engineered by the stacking order of the dielectric layers, which can form energy barriers generated by offsets in their respective valence and conduction band edges and/or through band bending at equilibrium. As these trapped charges travel through the dielectric layers and recombine to ultimately restore the flatband voltage, we seek to characterize their transport through the following measurements.

Initial characterization includes a multi-frequency capacitance-voltage (CV) measurement to study the interface trap density. Throughout ionizing radiation dosing, single high-frequency CV measurements are performed to evaluate the dependence of flat-band voltage shift on dose. After dosing, a series of CV measurements are performed as a function of time to analyze room-temperature annealing which yields information on the placement and movement of these charges.

Imaging Photonic Modes of a TiO2 Metasurface via Photoelectron Emission Microscopy

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Speaker: Andrew R. Kim

Nanophotonics seeks to precisely control light-matter interactions at optical and telecommunications wavelengths through resonant optical devices such as metasurfaces and photonic crystals, to exploit in sensing, imaging, and nonlinear optics. To this end, dielectric metasurface engineering has seen remarkable progress in confining light to sub-wavelength length scales by manipulating the spatial symmetry of the system. It is thus important to investigate the relationship between the symmetry of the resonance and the symmetry of the illuminating light (polarization and k-vector) at the sub-wavelength limit. We present a photoemission electron microscopy (PEEM) study of optical resonances in the ultraviolet to visible photon energy (Eph) of a metasurface consisting of a square lattice of TiO2 nanorods. This approach involves sub-wavelength spatial resolution imaging of electromagnetic field distribution using far-field illumination at normal incidence enabling control of polarization, photon energy, and incident configuration (k-vector). To date, the relation between PEEM images of dielectric metasurfaces and the local field distribution is unsettled due to uncertainty in the probing depth of PEEM and in the sensitivity limit of PEEM to the illuminating k-vector. Our work addresses these uncertainties by comparing PEEM images of the metasurface, which supports two resonances with different spatial symmetries overlapping in Eph, to simulated electric field profiles. The simulations agree well with PEEM measurements and reproduce the switching between the two photonic resonances as a function of Eph and visualize subtle effects of the momentum of the illuminating light equivalent to 0.2° incident angle variation. Furthermore, we derive the inelastic mean free path (IMFP) of 35 nm of very low kinetic energy (<1 eV) electrons by comparing the intensity distribution of PEEM and simulated images. The estimated IMFP is comparable to the feature size of the photonic nanostructures and establishes the sizeable probing depth for applicability of PEEM towards evaluating spatially-confined electromagnetic fields in each resonator volume.

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Process-structure-property effects of debinding and sintering for an additively manufactured silica

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Speaker: Lindsey Bezek

Functional applications for additively manufactured ceramic parts are currently limited by both material constraints and limited knowledge of process-structure-property relationships. One challenge for developing new ceramics for additive manufacturing (AM) is determining a post-process heating strategy (including debinding and sintering) that yields parts with sufficient mechanical strength while mitigating defects and unpredictable shrinkage. This work explores how modifying debinding and sintering parameters (e.g., temperatures, hold times, and rates) affects material and mechanical properties of parts fabricated using a commercial silica-based resin and the vat photopolymerization AM process. Parts were qualitatively assessed for effective debinding, and parts were subjected to different sintering conditions to evaluate density, shrinkage, porosity, and flexural properties. Fundamental understanding of how post processing affects parts' structure and properties will enable establishment of guidelines on how to strategically select post-process conditions for new ceramics. This knowledge will facilitate predictable part performance and contribute to a framework to expand the applicability of ceramic AM parts for functional applications.

Electroplated LPBF and BPE Additive Manufactured 17-4 Stainless Steel

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Speaker: Natalia Saiz

Laser-Powder Bed Fusion (LPBF) and Bound Powder Extrusion (BPE) are additive manufacturing (AM) processes for metal that assembles in a layer-by-layer fashion. LPBF consists of metal powder that solidifies with laser. Meanwhile, BPE is similar to fused deposition modeling (FDM) and requires an external furnace to produce the desired component. Despite the advantages of AM, electroplating on additive manufactured surfaces have not been examined. The effects of electroplating metal AM components require further investigation. Electroplating demonstrates favorable surface enhancement qualities, however for AM processes such as LPBF and BPE these conditions have not been explored. In this work, we focus on electroplating LPBF and BPE 17-4 stainless steel. LPBF and BPE samples of 17-4 stainless steel are electroplated using different bath chemistries to achieve different thickness of Nickel-plated AM material. Results are discussed in the context of surface roughness along with tribological enhancements. These results show the feasibility of electroplating AM metal surfaces for potential adhesion, corrosion, and solder applications. The preformed Pin-On-Rod test determines the adhesion on the Nickel-plated LPBF and BPE samples. Based on the results, electroplated AM material properties are observed in a detailed study.

Post-Processing Techniques for AM Metals

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Speaker: Mary Louise Gucik

Over the past decade, additive manufacturing has emerged as a competeitive alternative to traditional fabrication; however the as-printed surface roughness greatly degrades surface sensitive properties requiring a post-processing step before integration for the intended use. A crucial question then becomes, which post-processing technique is appropriate for the part in question? Herein, results from mechanical and chemical techniques will be shared and the differences highlighted. Media blasting was investigated on AM parts with high aspect ratio geometries; variations in surface feature removal were interrogated with different types of media. Conversely, the brightening, smoothing, and deburring of metallic AM parts was chemically investigated through electropolishing. Environmentally friendly baths were targeted for traditional wet electropolishing work in constant and pulsed potential regimes and the results will be compared to commercially available dry electropolishing systems.

Additively Manufactured Mixed Potential Sensors for Methane and Hydrogen Emissions Monitoring

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Speaker: Lok-kun Tsui

Methane emissions from natural gas infrastructure contribute to global climate change and has a global warming potential 28x that of CO2 on a 100 year basis.[1] Moving hydrogen-methane blends in existing natural gas pipelines have been proposed as way to transport hydrogen for the deployment of the hydrogen economy.[2] For this to be feasible, sensors that can provide continuous monitoring are required for detection of leaks to minimize the environmental and safety impacts from hydrogen-methane blend transportation. Mixed potential electrochemical sensors are a solid-state sensor technology where the difference in catalytic activity of multiple dissimilar electrodes is used to sense gases. We have developed a process to prototype the sensors by direct write extrusion additive manufacturing of ceramic substrates, metal and metal oxide electrodes, and a porous solid-state electrolyte. The sensors consist of a magnesia-stabilized zirconia substrate, a porous yttria-stabilized zirconia electrolyte, and electrodes of indium tin oxide, La0.87Sr0.13CrO3, Au, and Pt. The additive manufacturing process was successfully transitioned to a traditional manufacturing method suitable for mass production, tape casting and screen printing. Mixed potential sensors exhibited a lower limit of detection of 3 ppm of CH4 and < 1 ppm for H2. The sensors were integrated into an internet of things package providing data readout and transmission to the cloud. The sensor packages were field tested at Colorado State University's Methane Emissions Technology Evaluation Center (METEC).[3] We demonstrated that above ground emissions of H2 at an emission rate of 2.0 SLPM could be detected at greater than 9 meters.

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A New Processing Parameter Paradigm for Blown Powder Laser Beam Directed Energy Deposition (L-DED)

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Speaker: Brett Tucker Roper

Laser beam directed energy deposition, or L-DED, is a melt based additive manufacturing (AM) process. Sandia has a home-built L-DED system, also known as laser engineered net shaping (LENS), in which powder flows in a stream coaxially with a laser in order to melt the powder and build up parts in a layer-by-layer fashion. In this talk, the development of a new paradigm for processing parameters is discussed. A new, more selective pre-build analysis allows for the efficient determination of informed process parameters for full builds. By optimizing and characterizing the laser, depositing single melt tracks, and building single layer depositions, more informed build parameters, such as optimal laser power input, hatch spacing, and layer height, can be determined. Other in processing conditions such as oxygen content within the build chamber and powder flow rates were evaluated and improved upon. The systematic characterization and optimization efforts contribute to advancing the technology and expanding its applications in various fields, ensuring higher-quality outcomes.

The Effect of Processing Parameters on the Microstructure and Mechanical Behavior of Ti5553

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Speaker: Austin Olivier

Titanium-5Al-5Mo-5V-3Cr (Ti-5553) is a metastable β-Titanium alloy that is a promising candidate for high strength aerospace structural components, such as landing gear and other load bearing components.1, 2 Recently, this alloy has also gained attention in the additive manufacturing (AM) community due to its low residual stress post-printing and heat treatability. This work investigates the effects that various processing parameters have on the alloy's microstructure and the resulting mechanical properties for AM and wrought Ti-5553. Post-print processing performed on the parts includes various heat treatments and welding on heat treated parts. Heat treatments on both conventionally manufactured and AM Ti-5553 can be used to tailor the mechanical properties for strength or ductility. In wrought Ti-5553, it was found that transformed beta in a globular alpha matrix had a positive effect on the ductility and martensitic alpha led to improved strength of the material. For AM Ti-5553 the as-built condition exhibits exclusively large beta grains and relatively poor strength, however post-build heat treatments can be used to achieve similar strengths to wrought material through microstructural transformations. Welding was shown to create large beta grains in the weld zone that exhibited lower strength and ductility than the parent material.

The Effect of Microstructure on Thermal and Electrical Conductivity of 14WYT NFA

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[1]University of New Mexico
[2]Los Alamos National Laboratory
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Speaker: Jared Justice

14YWT NFA samples consolidated by either Hot Isostatic Pressing or Hot Extrusion were produced at various temperatures to establish processing-structure-property relations. Microstructure investigation showed significant differences in grain size and structure. HIP processed specimens showed equiaxed grains with a bimodal distribution and increasing average grain size with increasing HIP temperature. The ER specimen showed a bimodal grain distribution with grains elongated in the extrusion direction. The electrical and thermal conductivity for nanostructured 14YWT was measured over a range of temperatures. Electrical resistivity was measured from 3 K to 400 K and thermal conductivity was measured from 300 K to 1275 K. Electrical resistivity proved to be highly sensitive to processing pathway, however thermal conductivity was microstructure independent. Other thermal properties including heat capacity, thermal diffusivity, and thermal expansion coefficient are also reported.

Oxygen Non-Stoichiometry and Thermochemical Hydrogen Production in Novel Machine Learned Oxides

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Speaker: Tyra C. Douglas

Solar thermochemical hydrogen production (STCH) is a promising approach to convert water into hydrogen by harnessing solar thermal energy, as opposed to using electricity in electrochemical methods. This process involves two steps: initially, a material undergoes thermal reduction at elevated temperatures (~ 1300 - 1500 °C) under low oxygen partial pressures (pO2) of ~10^-3 - 10^-5 atm, creating oxygen vacancies. Subsequently, the temperature of the system is reduced to ~800 - 1000 °C in the presence of steam, which facilitates water splitting through material oxidation. The commercial feasibility of STCH is dependent on identifying a material with an optimal reduction enthalpy that supports both the thermal reduction of redox-active cations and their re-oxidation, along with high cycle stability. Perovskite metal oxides have received significant interest as potential STCH materials due to their ability to accommodate high concentrations of oxygen vacancies and their highly tunable thermodynamic properties. However, these materials often exhibit low hydrogen production due to re-oxidation and poor cycle stability challenges. [1,2, 3]

Our team has developed a machine learning algorithm to identify materials suitable for STCH applications. [4] Utilizing the algorithm's predictions, we have focused on exploring compounds with redox-active cations beyond the commonly studied first-row transition metals such as Fe, Co, and Mn. From the thousands of compounds predicted by the model, we have selected candidates based on criteria for oxygen vacancy formation energy and stability. In this presentation, we will discuss the oxygen vacancy concentrations of selected compounds, derived from thermogravimetric measurements conducted at 10^-5 - 1 atm pO2 and temperatures ranging from 1000 °C to 1450 °C. We will also present an analysis of point defect equilibria and hydrogen production data obtained from flow reactor experiments. Comparisons with existing high-temperature experimental and modeling studies will be included to provide context and validation for our findings.

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Effects of External Magnetic Field on Mechanical properties and irradiation resistance of F/M Steels

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Speaker: Xiatong Yang

Ferritic/Martensitic (F/M) steels are one of the most promising candidates for structural and cladding applications in advanced reactors due to their better thermal properties and resistance to swelling compared to conventional austenitic stainless steels. However, F/M steels suffer from radiation embrittlement at low temperatures (<400°C), creep at elevated temperatures (>500°C) and swelling at very high irradiation doses at intermediate temperature ranges (400-450°C). Tempering under external magnetic field has the potential to address these challenges by engineering the microstructure including the size and morphology of carbides. In this study, we will present an overview of magnetic field effects during tempering followed by our recent findings showing the effects of external magnetic field on the microstructure and mechanical properties as a function of magnetic field strength of up to 9T. The specimens tempered with and without external magnetic field are characterized using electron microscopy based techniques together with transmission electron microscopy on selected alloys and will also be subjected to light and heavy ion irradiations in the future.

A direct upcycling approach for spent lithium ion battery materials via microwave exfoliation

Clare Davis-Wheeler Chin[1],
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Speaker: Clare Davis-Wheeler Chin

Rapid market growth of lithium ion-batteries (LIB) for electric vehicles has generated critical materials and sustainability challenges. LIB cathodes require cobalt, which is costly and primarily mined in conflict regions. In response, recent efforts focus on developing efficient, scalable methods for recycling spent LIB cathode materials. Here we report a direct-upcycling approach that exploits microwave (MW) heating for exfoliating layered cathode oxides LiCoO2 (LCO) and LiNixMnyCozO2 (NMC) into nanosheets (NSs), which facilitates manipulation of Co:Ni:Mn stoichiometry and reassembly into functioning cathode materials. MW irradiation interacts directly with reaction species to promote heterogeneous heat distribution and instantaneous localized superheating, accelerating exfoliation rates and increasing conversion from bulk oxides to NSs. Our “one-pot” MW method decreases exfoliation time from 2 days (leading-edge electrochemical method) to 2 hours and is easily scaled to generate multi-gram yields. High-resolution transmission electron microscopy (HR-TEM) of MW-exfoliated LCO and NMC indicates conversion into mono- and bilayer NSs with significantly higher yield (>95% vs. 60%) vs. electrochemical exfoliation. Analysis of NSs lattice fringes (supported by X-ray diffraction spectroscopy) demonstrates good crystallinity and absence of undesirable phase conversion. The results of this work help establish a fundamental science foundation for sustainable scale-up and securing the LIB supply chain, which is a DOE priority.

Development and Construction of Liquid Lead-Lithium Loop at UNM

Xavier Angus[1], Sergey Smolentsev[2], Bruce Pint[2], Marie Romedenne[2], Claude De lamater-Brotherton[2], G. Ivan Maldonado[3], Nick Brown[3], Quang Son[3], Michael Trombetta[1], Daniel Levario[1], Osman Anderoglu[1]
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Speaker: Xavier Angus

Liquid lead-lithium eutectic is one of the potential coolants for use in blankets of fusion reactors due to its favorable heat removal properties and its high tritium breeding ratios relative to other coolants. However, lead-lithium is highly corrosive and will be subjected to high extreme magnetic fields resulting in pressure drops known as magnetohydrodynamics (MHD). Studying the challenges associated with lead-lithium eutectic, especially structural materials compatibility of liquid lead-lithium is necessary to ensure the long-term viability of a lead-lithium-cooled blanket.

This project involves the design and construction of a forced convection lead-lithium loop out of SS316 to test corrosion rates at high flow rates (up to 1 m/s) and temperatures (up to 500° C) in the presence of an external magnetic field. The key components of this loop include removable tubing sections for inserting test material, a high-powered electromagnet (~2T), and a capacity of three gallons of lead-lithium. The electromagnet enables pressure drop studies and corrosion tests at high magnetic fields, simulating the environment in a blanket. The loop also incorporates various instrumentation such as a Venturi flow meter and differential pressure sensors for MHD and flow accelerated corrosion studies.

The modular design of the loop allows for comprehensive testing and easy replacement of components, facilitating long-term studies of material behavior within the simulated environment. This setup aims to provide critical data on corrosion behavior and MHD effects in high-temperature liquid lead-lithium environments, contributing to the ongoing development of lead-lithium as a fusion reactor coolant.

Designing New Materials Based on Barium Niobates For the Electrochemical Oxidative Coupling of Methane

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University of New Mexico, Albuquerque, NM 87131, USA.

Speaker: Kanna Ramaiyan

****INVITED SPEAKER****

Methane is the major component of natural gas and recent discoveries of new natural gas resources has made methane a cheap source of energy. Methane is also a greenhouse gas (GHG) with a global warming power that is 21 times higher than that of CO2 and is often flared or released to the atmosphere from smaller oil and gas fracking wells where methane extraction is economically unfeasible. Hence, effective conversion of methane into value added chemicals such as ethylene will help reduce methane emissions and is a major research area for the past 40 years. Oxidative coupling of methane (OCM) at elevated temperatures is shown to produce ethylene although over oxidation products such as CO2 and CO reduce the C2 hydrocarbon selectivity. The industrial target for OCM process is a single pass conversion of at least 30% and a C2 selectivity around 80% although catalysts with satisfactory performance has not been identified.1 Electrochemical OCM in solid oxide electrolyzers is recently gaining renewed interest due the ability to control the conversion rate and product selectivity though temperature and applied potential. However, high temperature operation also leads to materials degradation via sintering, crystal structure disproportion to thermodynamically more stable phases, and interfacial reactions that reduces the performance.

We have developed an exciting class of barium niobate perovskite materials with varying level of Mg/Ca doping along with one or more of Fe, Ni, Co, and Y co-doping for methane activation in the electrochemical and conventional oxidative coupling environment.2-5 This class of perovskites show exceptional chemical stability and catalytic activity under OCM measurements. The reason for the catalytic activity, chemical stability and electrical properties have been analyzed using various physical characterization techniques such as thermogravimetric analysis, PXRD, XPS, temperature programmed reaction measurements, chemisorption measurements, along with electrochemical characterizations to rapidly determine their stability under operationally relevant conditions and these results are compared to stability calculations. OCM measurements with our catalysts reach the industrial target and optimization is underway to exceed the target. These perovskite materials could also serve as a support for a wide variety of catalyst materials for high temperature applications thus opening up new possibilities.

Stability analysis of Single Atom Platinum Catalyst synthesized using a Plasmon-enhanced method

Hirithya Sharad Jeyashangararaj[1], Naomi Helsel[1], Xuan Pham[1], Dr. Corey Leclerc[1], Dr. Pabitra Choudhury[1], Dr. Sanchari Chowdhury[1]
[1]Dept of Chemical Engineering, New Mexico Institute of Mining and Technology

Speaker: Hirithya Sharad Jeyashangararaj

Single-atom Pt catalysts and Pt nanoclusters deposited on Titanium nitride are promising catalysts for different reactions such as hydrogen evolution reaction, CO oxidation and methanol oxidation. We have successfully deposited size controlled single atom platinum catalyst (SAC) and Pt nanoclusters on refractory plasmonic titanium nitride (TiN) nanoparticles using visible light. Titanium nitride nanoparticles can absorb broad spectrum solar light to generate photoexcited electrons which reduce Pt precursor salt to deposit as metal atoms on the surface. SACs are atomically dispersed metal atoms, and though they have high efficiency, they also have high surface energy that can lead to instability through aggregation or sintering. DFT calculations are performed to investigate interactions between Pt and TiN such as binding energy and aggregation energy of Pt on different sites of TiN. The calculations suggest that strong metal-support interactions between Pt and TiN help in anchoring the single Pt atoms on TiN, reducing their mobility and preventing aggregation. Under severe temperatures or in reactive conditions, these interactions may weaken, leading to the aggregation of the metal atoms. To understand the stability of the synthesized TiN supported single Pt atoms as well as Pt clusters, we are investigating the sintering processes of the catalysts by exposing them to high temperature. In addition to using high resolution transmission electron microscopy to study the size and structure change of catalysts upon sintering, XPS studies have been employed to examine the metallic states of the catalysts which are crucial to evaluate their catalytic efficiency. We are studying the hydrogen adsorption properties of our fresh catalyst as well as catalysts sintered at different temperatures to understand the effectiveness of the catalysts for the reactions such as hydrogen evolution reaction and hydrogenation reactions. The variation in the capability of hydrogen adsorption is observed when there is aggregation or sintering.

A new approach to the surveillance of electronic components and circuits

Thomas Buchheit[1], Paul Kuberry[1], Biliana Paskaleva[1], Andrea Jin[1], and Ting Mei[1]
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Speaker: Thomas Buchheit

Traditionally, compact analytic device models are used to simulate the electrical behavior of discrete electronic parts in circuits. These models require subject matter experts with proprietary tools to perform calibration from collected data. Though traditional compact models have application in understanding the physics which drive device behavior, their idealized expressions do not precisely represent observed data. Furthermore, compact models might not be sufficiently accurate and sensitive to be useful for tracking changes in component's behavior due to aging. To overcome these limitations, we have developed a data-driven modeling interface, Xyce-PyMi, for directly incorporating part-level data collected in the field or laboratory into Sandia's Xyce circuit simulator. An interface tool that provides an exact replication of discrete part electrical behavior, which can capture subtle changes due to part-to-part variability or aging. Details of exploiting the Xyce-PyMi Python-based modeling interface to create either DC or transient electrical measurement models from data collected on discrete electronic parts, specifically diodes, bipolar junction transistors and MOSFETS will be given. Application of the data-driven part models in prototype test circuits will be addressed in the final part of the presentation.

Carrier Lifetime Control Through the Quantum Confined Stark Effect

James Loveless[1], Vincent Meyers[1], Anthony Rice[1], Mike Smith[1], Luke Yates[1], Robert Kaplar[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: James Loveless

The manipulation of minority carrier lifetimes in III-N quantum wells (QWs) through the quantum confined Stark effect (QCSE) presents a promising avenue for optimizing semiconductor device performance. This study investigates the impact of well width on carrier lifetime, revealing a nuanced interplay between charge separation and screening effects. As the QW width increases, the spatial separation of electron-hole pairs due to QCSE enhances the radiative lifetime. However, as the well width continues to increase, the charge screening effect becomes more prevalent, counteracting the internal field and effectively flattening the potential in the wells. As the charge separation effect diminishes, the carrier lifetime is reduced, transitioning into bulk-like behavior. Numerical analysis shows a peak of carrier lifetime at a QW width of approximately 20 nm, while QWs with a width of 50 nm show no enhancement of lifetime, similar in magnitude to narrow QWs of approximately 1 nm.

To validate the numerical analysis, time-resolved photoluminescence (TRPL) was performed on several superlattice samples of varying sizes, ranging from 40 nm to 80 nm. These measurements showed good agreement with the numerical study, however, current test structures have all fallen opposite the peak in the charge screening regime. Additional structures (10 nm to 40 nm well widths) will be evaluated to provide understanding of peak lifetime enhancement and reduction as the charge separation is reduced. Photoluminescence (PL) measurements will be used to further corroborate these findings through the observation of a red-shift in transition energy for samples where the QCSE is prevalent. As the carrier density is increased through excitation power, the charge screening effect is amplified, and the red-shift in transition energy should effectively disappear.

The ability to tailor carrier lifetimes through precise control of QW dimensions has significant implications for various semiconductor applications. One notable application is in photodetectors, where extended carrier lifetimes can improve sensitivity and signal-to-noise ratio. This work not only enhances our understanding of QCSE in III-N QWs but also opens pathways for designing advanced optoelectronic and power devices with customized carrier dynamics.

Remote Epitaxy on Nonuniform Surfaces and the Influence of Imperfections

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Kevin S. Jones[2], Scott W. Schmucker[1]
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Speaker: Manny X de Jesus Lopez

The field of remote epitaxy involves crystal growth where the substrate and epitaxial film are separated by a graphene monolayer. The presence of this graphene layer prevents direct covalent bonding between the film and the substrate, enabling transfer for heterogeneous integration and improving film quality. We will explore the origins of remote epitaxy and the competing influences of pinholes, substrate imperfections, and contamination on the epitaxial growth process.

Remote epitaxy is often assumed to proceed on a pristine material stack, free from imperfections. However, in real systems, through-graphene epitaxial growth may proceed by multiple processes which occur in parallel. Depending on the material system, remote epitaxy can occur above a pristine graphene monolayer. However, if pinholes exist in the graphene the nucleation may occur directly on the substrate and single-crystal films may result from pinhole-mediated lateral overgrowth. This is a competing epitaxial growth process to remote epitaxy. It is also possible epitaxy may be inhibited by contaminants above or below the graphene monolayer, or by the presence of bilayer or few-layer graphene islands.

Previous studies have demonstrated the potential of remote epitaxy for high-quality film growth and substrate reuse. However, the influence of pinholes on the epitaxial process remains underexplored. Earlier works have suggested that pinholes can either facilitate or hinder epitaxial alignment. Researchers have observed each of these competing influences in experimental studies, but no detailed understanding of the relative influence of each has been developed.

This study builds on these findings by providing a systematic analysis of pinhole effects, aiming to isolate the contributions of epitaxial lateral overgrowth and remote epitaxy in the presence of such imperfections. Specifically, we aim to define the role of pinholes by systematically varying their size and density to assess their impact on epitaxial growth. Here we simulate the initial stages of epitaxial growth to develop a predictive capability for contributions from remote epitaxy and lateral overgrowth as a function of the density and nature of specific imperfections in the graphene overlayer. This study will drive a fundamental understanding of the early stages of remote epitaxial growth on imperfect surfaces in our future experimental studies.

Solder Joint Reliability in Fine Pitch BGAs

Hannah N Fowler[1], Jeier Yang[1], Joshua Minster[1], Deborah Hagen[1], Jessica Buckner[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Hannah N Fowler

Solder joint reliability is crucial to the functionality of electronic devices. Solder joint failures due to cyclic loading during thermomechanical fatigue or vibration are common sources of device failures, and, as we continue to expect higher performance out of our electronics, the problems with solder joint reliability continue to evolve. This can be seen in printed wiring assemblies and packages designed for increased interconnect density. Increased interconnect density means greater potential for increased computing power in a smaller footprint. Surface mount components, including fine pitch ball grid arrays (BGAs), allow for increased interconnect density. This study seeks to explore whether fine pitch BGAs, in this case with a ball to ball center distance under 1mm, may come with increased reliability concerns in thermal cycling.

Simulating dose-rate events on electronic parts utilizing high-power laser

Luke Packan[1], David Canfield[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Luke Packan

Assessing radiation effects on performance of electronic parts using a radiation source can be a lengthy and involved process. This assessment includes setting up a test plan, creating test boards, allocating time at a test facility, and factoring in time spent travelling. Radiation sources also uniformly hit both the device under test as well as accompanying cables and boards of the test setup. To alleviate some of these issues, the use of high-power lasers can simulate the effects of a radiation source without the negatives of the traditional path of radiation testing.

A high-power laser can be shot onto the exposed die of electrical parts to simulate the effects of dose-rate events. High-energy photons from the laser can generate free charge in the form of electron hole pairs as well as interface states in oxides. This trapped charge causes quasi-permanent device shifts leading to possible functional failure. An equivalent dose-rate model can be developed for the laser with comparisons of measured data for parts sent for radiation doses and 0the results from the same parts under fire by a high-powered laser. This would allow for simulating radiation effects at specific dose-rate levels by setting the laser to specific power and timing conditions.

In this presentation, we discuss the development of a 600-Watt, 808 nm laser system designed to simulate the electrical response of electronic parts to radiation dosage.

Evaluation of bend ductility in Ta-W alloys

Zahra Ghanbari[1], Christopher Finfrock[1], Christopher Murtagh[1]
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Speaker: Zahra Ghanbari

For various applications, tantalum (Ta) alloys are selected when it is important to maintain strength and ductility during and after a broad range of temperature and environmental exposures. Bend testing is a material efficient, method by which the mechanical properties of these alloys, particularly ductility and cracking susceptibility, can be evaluated post-exposure to complex environments. In this study, a guided bend test fixture was developed to test to a nominal 20% strain criteria on tantalum – 10 weight percent (Ta-10W) ring specimens. Bend testing of Ta-10W was performed on: as-received material, after heat treatment in atmosphere with controlled levels of oxygen (O), and after heat treatment in air. Thresholds in bend ductility were identified based on the presence or absence of cracking on the outer fiber of bend specimens. Light optical microscopy (LOM), scanning electron microscopy (SEM) were used to characterize the resulting cracks and propose ductility versus O-exposure relationships.

Antibacterial sustainable concrete with waste plastic and natural materials

Lukman Abubakar[1], Sameer Jain[1], Zayden Brieno[1], and Arjak Bhattacharjee[1]
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Speaker: Sameer Jain

Globally, concrete is the most often utilized building material. Ordinary Portland cement (OPC), made from carbonaceous raw materials at a very high temperature, is the main ingredient in concrete. This significantly contributes to global carbon emissions. United Nations Environmental Program (UNEP) encourages decarbonization of building and construction industries by implementing alternative sustainable materials. Hence, there is a growing demand to use waste materials for reinforcement in concrete. Because concrete is naturally brittle, environmental factors like humidity, temperature changes, rain, etc. can cause concrete structures to fracture and contaminate them with bacteria. Despite concrete's strength and durability, the risk of microbiological deterioration continuously puts it to the test. Sewage systems and coastal regions are ideal habitats for microbes because they are moist extremely humid and full of organic debris. These microorganisms can degrade concrete directly or cause reactions that compromise the concrete's structural integrity through the byproducts they produce. These bacteria have the potential to accelerate the concrete's disintegration, necessitating a large financial outlay for upkeep and restoration. The current work targets to address these issues. The objectives of this study are twofold, first is to fabricate antibacterial concrete using turmeric coating and the second is to use household plastic waste as a reinforcing material in the concrete for partial replacement of fine aggregates. The obtained results show that turmeric coating does not adversely affect the compressive strength of the concrete structures. Phase identification with X-ray diffraction (XRD) and differential scanning calorimetry (DSC) shows that the addition of turmeric does not cause any adverse effects. The addition of turmeric leads to ~ 68% antibacterial efficacy against S. aureus. A current study is underway to fabricate concrete structures with waste plastic as a partial replacement for the fine aggregates in the concrete. To successfully carry out this aim, one in-house plastic cutter is developed in our lab followed by the collection of household plastic bottles and cutting them into short strips. These will be used as a reinforcing material into the concrete.

Data-Driven Optimization of Interlocking Metasurface Design

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Speaker: Nathan Brown

****INVITED SPEAKER****

Interlocking metasurfaces (ILMs) are a new class of mechanical metasurfaces built from architected arrays of interlocking features that can serve as a nonpermanent, robust joining technology. An ILM's strength is governed by the constitutive material, orientation, and topology of its latching unit cells. The presented work optimized the topologies of ILM unit cells to maximize strength in tensile and shear loading using parametric optimization, genetic algorithms, and deep machine learning methods. Experimental validation confirmed that the optimized designs achieved considerable strength increases for isolated unit cells and arrays of interacting unit cells (metasurfaces) compared to a human intuitive design. This study compares how unique design methods can result in high-performing design solutions to maximize ILM effectiveness under single- and multi-objective scenarios. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Oxidation Behavior of Niobium and Tantalum-rich Refractory Complex Concentrated Alloys

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Speaker: Krishna Prasad Joshi

Refractory complex concentrated alloys (RCCAs) have shown significant promise for high-temperature applications due to their exceptional strength and thermal stability in elevated temperature regimes. However, the oxidation resistance of these alloys is a crucial factor for their suitability in such conditions. This study investigates the oxidation behavior of two novel RCCAs: Nb32.5Ta32.5Mo7.5W7.5V10Ti10 and Nb30.55Ta30.55Mo7.05W7.05V9.4Ti9.4Cr6, fabricated using a powder metallurgy process. Oxidation tests were conducted at 1000°C for 0.5, 5, and 10 hours, with performance comparisons made to the wrought C103 alloy. Noticeable oxidations were noted around 500°C for the C103 alloy and around 700°C for the RCCAs. At 1000°C, the C103 alloy exhibited a linear weight increase per unit area over time. In contrast, the RCCAs demonstrated a parabolic weight gain per unit area that decreased with time, indicating a more protective oxide layer. Among the RCCAs, the alloy containing chromium (Cr) exhibited the lowest oxidation rate. The oxidation kinetics of C103 at 1000°C revealed a linear oxidation rate, while the RCCAs showed a time-dependent reduction in oxidation rate, especially for the Cr-containing alloy. The oxidation behavior of these RCCAs will be discussed with respect to the composition and structure of the oxide layers formed during exposure to high temperatures.

Effects of Environmental Species on Tribological Properties of MoS2: Using Simulations to Interpret Experimental Observations

N. Scott Bobbitt[1], John Curry[1], Tomas Babuska[1], Michael Chandross[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Scott Bobbitt

****INVITED SPEAKER****

Molybdenum disulfide (MoS2) is a lamellar solid with applications in semiconductor devices, catalysis, and lubrication. The layers of MoS2 interact via weak van der Waals forces, enabling the layers to slide with a low coefficient of friction in dry or vacuum environments. This makes MoS2 an attractive solid lubricant for use in satellites and other aerospace applications. However, exposure to environmental species, e.g. oxygen and water, has been shown to degrade the lubricating properties of MoS2. The precise mechanisms of the interactions between MoS2 and water and how these interactions affect its tribological properties remain poorly understood. In this talk, we will present our theory for how adsorbed water impacts the tribology of MoS2 lubricants, based on experiments and simulations. We report the coefficient of friction over a wide range of humidities using vacuum-based tribological experiments and describe how different types of molecular simulation (density functional theory, Monte Carlo, and molecular dynamics) augment our interpretation of those experiments. We will present computed adsorption isotherms for water adsorption on MoS2 under realistic atmospheric conditions We will discuss the interaction of water and oxygen with common defects in MoS2, including sulfur vacancies, edge defects, grain boundaries, and oxidized sites. Finally, we will discuss how water adsorption on MoS2 impacts the tribological performance of the material.

Resolving local structure in alloys through thermodynamic ensembles of pair distribution functions

Vanessa Meschke[1], Andrew Novick[1], Jen Rogers[2], Claire Porter[1], Remco Chang[2], Thomas Proffen[3]
Eric S. Toberer,
[1]Colorado School of Mines
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[3]Oak Ridge National Laboratory

Speaker: Vanessa Meschke

Characterizing local bonding environments in complex materials is essential for understanding and optimizing their properties. Equally as important is the ability to predict local motifs as a function of synthesis conditions, enhancing chemists' ability to design properties into materials. In this study, we present an approach to leverage statistical mechanics to generate temperature- and energy-informed ensemble averaged pair distribution functions (PDFs). This method, which we have named Thermodynamic Ensemble Averages of PDFs for Ordering and Transformations (TEAPOT), utilizes density functional theory (DFT) to relax supercells while incorporating energetic penalties for local order, enabling accurate and computationally efficient analysis of local structure. We apply this method to the neutron PDF measurements of the pseudobinary MnTe-GeTe (MGT) alloy, demonstrating its capability to resolve complex local distortions and chemical ordering. Our results reveal detailed insights into phase transformations and local distortions driven by Mn substitution. For compositions that globally present as rock salt, our analysis reveals that Ge coordination geometry is heavily impacted by synthesis temperature. We propose that high temperature synthesis conditions promote a lowered Ge polyhedra distortion, promoting high charge carrier mobility due to the alignment of local and global structure. Incorporating statistical mechanics and computation into experimental analysis thus guides synthesis of tailored local structure.

Structural and electronic properties of structural refractory binary alloys

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[3]Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131

Speaker: Surya T. Bijjala

Exploratory alloy discovery, design, and development are crucial aspects of materials research. Refractory high-entropy alloys (RHEAs) with 5+ elements, mixed in near equiatomic fashion, represent an exciting class of structural materials with the potential for achieving combined ductility (manufacturability) and high strength in refractory systems. However, exploring the vast number of possible compositionally-complex RHEA alloys in order to optimize their respective mechanical properties is a significant challenge. Machine learning (ML) techniques utilizing first-principles descriptors may enable efficient exploration of this large design space, based on a high-quality dataset of unary and binary counterparts. We have performed comprehensive DFT calculations for the relevant unary and binary systems to investigate the interplay between electronic correlations and atomic disorder in these systems, and establish an appropriate training dataset for predicting the properties of complex alloys. We present results for structural properties, formation enthalpies, and the electronic structure of MoNb, MoTa, MoW, NbTa, WNb, and WTa BCC refractory binary alloys as a function of alloy composition, computed using the ABINIT electronic structure code. Initial benchmarking studies were performed to establish the methodology and computational parameters for Mo, Nb, Ta, and W. Computed properties using d, p, and s valence electron-norm-conserving pseudopotentials and using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation energy density functional agree well with other theoretical calculations and with experiment. Special quasi-random structure (SQS) supercells were used to represent the disordered binary alloys. The effect of strain due to the random arrangement of atoms of different atomic radii in SQS supercells was studied by considering spin and relaxation effects on structural properties.

Mesoscale Modeling of Fiber-Reinforced Composites for Marine Energy Environments

Peter J Creveling[1], Evan M Anderson[1], Bernadette A Hernandez-Sanchez[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Peter J. Creveling

Fiber-reinforced composites (FRCs) are an attractive material system within tidal energy converter systems due to their unique material properties in marine energy environments, including high specific strength and stiffness, corrosion resistance, and tailorable material properties due to the anisotropic behavior of the fibers. Accurately quantifying the performance of these materials within existing and future systems in these environments is challenging due to the manufacturing defects (e.g., cracks and pores), variation in constituent (i.e., fibers and resins) material properties among manufacturers, and evolution of constituent properties between dry and fully saturated states.

This study seeks to address the above challenges by first developing a mesoscale model of an ideal FRC geometry in which input constituent material and geometric property ranges are collected from both experimental data and existing literature and used to make estimates of output mechanical and diffusive quantities of interest. Of particular interest are effective elastic moduli, diffusivity and coefficients of moisture expansion for the composite. From the range of model input parameters, an uncertainty quantification and sensitivity analysis study is performed by quantifying which input parameters greatly influence the output response through calculation of Sobol' indices, and which set of input parameters best agrees with experimental data. Next, imaged-based simulations are performed to model moisture uptake with respect to time. The geometry is constructed from X-ray computed tomography images of FRCs such that manufacturing variability and defects are explicitly represented within the model. Results from the analytical model are ultimately used to inform model input parameters for imaged-based simulations, and initial results show good agreement with experimental data. This work was funded by the DOE Energy Efficiency and Renewable Energy, Water Power Technologies Office program. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Evaluation of Ba(Al,Fe)2O4, a Machine Learned Compound, for Solar Thermochemical Hydrogen Production

Sean R. Bishop[1], Matthew D. Witman[1], Keith A. King[1], Arielle L. Clauser[1], Perla A. Salinas[1], Andrew Rowberg[2], Joel Varley[2], Tyra C. Douglas[1], Stephan Lany[3], Anuj Goyal[3], Joshua D. Sugar[1], Eric N. Coker[1], Tadashi Ogitsu[2], and Anthony H. McDaniel[1]
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[3]National Renewable Energy Laboratories

Speaker: Sean Bishop, Staff Scientist

****INVITED SPEAKER****

Solar thermochemical hydrogen (STCH) production uses concentrated sunlight to produce hydrogen using reduction/oxidation of metal oxides. Typically, the metal oxide is heated to high temperature (>1400 oC) causing it to release oxygen, then it is cooled to a lower temperature (~<1000 oC) in steam whereby it re-oxidizes, stripping oxygen from water molecules and producing hydrogen. Due to improved stability, non-stoichiometric oxides that do not change phase during the STCH process are typically used, even though the reversible oxygen content is less than phase changing materials. In this presentation, recent progress in developing a new water splitting material based on BaFe2O4 will be presented. The composition was predicted to exhibit attractive STCH performance by a defect Graph Neural Network trained on crystal structures derived from density functional theory. Overcoming temperature instability by partial Fe substitution with Al will be discussed. Characterization of high temperature oxygen release using thermogravimetric analysis, hydrogen production from flow reactor measurements, and pre and post-test advanced electron microscopy will be presented. Additionally, atomistic simulations providing insight into defect structure will be discussed.

Analytical Electrochemistry of Nickel and Platinum Electrolytes

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[1]University of New Mexico
[2]Sandia National Laboratories, Albuquerque, NM

Speaker: Kyle Troche

Pt-Ni alloys possess unique catalytic and magnetic properties, and it is highly desirable to synthesize conformal thin films of these materials for integration into magnetic devices and energy conversion systems. Electrodeposition provides large scale and complex form plating without the need for additional equipment such as a vacuum system or furnace used in traditional Pt-Ni synthesis. While nickel and platinum electrodepositions can individually plate effectively, co-deposition provides its own challenges. Two major challenges need to be addressed, the large differences in deposition potentials between the two metals and platinum's reduced overpotential for undesirable hydrogen evolution. Investigation into various nickel and platinum bath chemistries over a range of pH's will help develop a Pt-Ni co-deposition bath that will produce a uniform deposition with desired morphologies. A rotating disk electrode experiment was conducted on each electrodeposition bath along with a Koutecky-Levich analysis to determine the baths diffusion coefficient and rate constant. Nickel baths include boric acid, acetic acid, citric acid, hydrochloric acid, and phosphoric acid. Platinum baths include hydrochloric acid and acetic acid. Hydrogen suppression techniques were also studied for both nickel and platinum baths to determine the effect on hydrogen generation and metal deposition. Successful suppression of the hydrogen generation reaction would result in greater control of nickel deposition onto platinum as well as thicker platinum films.

Predicting the corrosion rate of 316L stainless in 10 M HCl.

ThankGod Nwokocha[1] & T. David Burleigh[2]
[1]Intel Corporation, Rio Rancho, NM
[2]New Mexico Tech

Speaker: ThankGod Nwokocha

Containers made from 316L stainless steel are used to store radioactive waste. Radiolysis of the polyvinylchloride polymer inside these containers produces hydrochloric acid which corrodes the 316L stainless steel. It would be very useful to be able to predict the lifetime of these 316L containers in the presence of HCl. Various electrochemical and weight loss tests were used to understand the corrosion rate. The longest tests were 100 days. The observation was made that the longer the test was conducted in 10 M HCl, the faster the corrosion rate became, and the shorter the predicted lifetime. This implies that the HCl is continually degrading the passive film, making it more susceptible to corrosion.

Effect of Pore Shape on Collapse Behaviors in Explosives

Kerry-Ann M. Stirrup[1], Wayne W. Chen[1]
[1]Sandia National Laboratories. Albuquerque, NM

Speaker: Kerry-Ann Stirrup

The study of failure mechanisms in explosive materials under shock conditions is crucial for accurately modeling initiation and hotspot formation behaviors. The presence of naturally occurring flaws - such as inclusions, cracks, and porosity - significantly influences the fracture behavior of these materials. Traditionally, experimental investigations have been limited to simpler geometries, like cylindrical pores, due to machining constraints. However, advancements in Focused Ion Beam (FIB) milling have revolutionized this field by enabling the creation of more intricate and realistic flaw geometries.

Harnessing Carbon Dots for Multifunctional Materials: From Synthesis to Applications

Koushik Ghosh[1], John Grey[1], Terefe Habteyes[2], Keith Fritzsching[1], Michael Holtzman[1], Kenneth Plackowski[1]
[1]Sandia National Laboratories, Albuquerque, NM
[2]University of New Mexico

Speaker: Koushik Ghosh

****INVITED TALK****

Carbon dots (CDs), an organic counterpart of quantum dots, have garnered significant attention due to their exceptional optical properties, photostability, and quantum confinement effects. Synthesized via top-down or bottom-up approaches, CDs offer a versatile platform for various applications. This study focuses on the bottom-up synthesis of CDs using urea and citric acid as two naturally abundant precursors. We demonstrate how molecular heterogeneity within the reaction mixture can be exploited to engineer CDs with tailored properties for humidity sensing. Additionally, the excitation-dependent emission of CDs is leveraged for sensing applications. The temporal evolution of the reaction mixture is explored to reveal self-assembly phenomena, leading to the formation of complex structures. In-depth structural investigations are conducted to establish a structure-function relationship, dispelling misconceptions about CDs and paving the way for the development of multifunctional materials. Our findings underscore the potential of CDs as a promising class of materials with diverse applications.

A Bidirectional Reciprocating Experiment for Macroscale Friction Measurement

Matthew Swanson[1], Brendan Nation[1], Jonathan Leonard[1], Christine Roberts[1], Sharlotte Kramer[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Mark Foster

The friction between the internal components of engineered systems, where components are installed into assemblies with polymeric protection materials, affects both the assembly process and the mechanical behavior of the system in operational and accident scenarios. Unfortunately, the frictional behavior of different material pairs is not well characterized in compression, even though that knowledge is vital to credible computational simulations of these systems in vibration, impact, or shock environments. An experimental method was developed to examine load-dependent, macroscale friction behavior between material pairs from an exemplar assembly. The materials of interest here were PMDI rigid foam, Sylgard 184, aluminum, and a silicone-based direct-ink-write lattice material. Utilizing a custom fixture that enabled simple exchange of materials, two horizontal actuators applied an even compressive load to the material pairs, and a vertical actuator cyclically displaced one of the materials relative to the other. Results indicated reversible behavior independent of slip direction, and maximum friction coefficients were compared to steady state friction behavior. Also, compressive load greatly affected the friction between some material pairs, but not all. This presentation will describe the novel experimental method and the frictional behavior of several pairs of dissimilar materials. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Monitoring impact of photothermal heating on light induced Diel's-Alder reaction: Thermoset recycle

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Speaker: Arnob Dipta Saha

Due to superior mechanical properties, high chemical resistance, and outstanding thermal stability, thermosets are highly suitable for a diverse range of applications such as adhesives, electronics, automobiles, aerospace, and household devices. However, the recycling of thermosets has posed a significant challenge due to their irreversible crosslinked structure limiting their reprocessability and recyclability. This study involves the incorporation of refractory plasmonic photothermal Titanium Nitride (TiN) nanoparticles into epoxy modified by Diel-Alder reaction. These nanoparticles can absorb light and generate localized nanoscale and macroscale heat, respectively. This heat can then drive reversible reactions, such as Diels-Alder reactions, which enable the recycling of the epoxy material. Nanoparticles loading and their dispersion in the polymer matrix is optimized to maximize their photothermal efficiency. We used in situ FTIR to study the kinetics of both forward and reverse Diels Alder reactions driven by photothermal effects and compared that with conventional heat driven reaction kinetics. One of our major observations is that, despite the sample having a similar bulk temperature, the forward Diels-Alder reaction kinetics with light-induced photothermal heat generation varies dramatically from conventional heating. To the contrary, the kinetics of the reverse Diels-Alder process was not significantly altered by the presence of nanoparticles and different stimuli. It implies that the Diels-Alder reactions may be impacted differently by reactant interaction with nanoparticles and local heat generation surrounding the nanoparticles. Further investigation of the system revealed that, while the dienophile remains unaffected by light or heat stimuli, the furan diene precursor can undergo crosslinking by reacting with singlet oxygen produced due to photosensitizing effect of TiN nanoparticles.

Hydrogen Diffusion In Oversaturated EPDM Rubber: The Effect Of Induced Strain

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Speaker: Hannah Dedmon

The development of hydrogen based energy and associated storage and distribution has lead to an infrastructure dependent on an advanced understanding of hydrogen materials interactions. To contain the high pressures associated with compressed hydrogen gas, multi-material components are crucial, of which polymers are used for parts such as O-rings, pipes, hoses, and inner liners of high pressure tanks. Although polymers are chemically inert when exposed to hydrogen gas, the cyclic pressurization and depressurization of hydrogen through polymer materials prompts mechanical failures. Previous experimental and computational works have explored the rapid decompression failure of rubbers leading to an understanding of polymer deformation as a function of hydrogen diffusion. However, we hypothesize that the diffusivity of hydrogen in rubber is influenced by local strain of the elastomeric material requiring an atomistic scale inquiry and description. In this work we establish a method to study hydrogen diffusion in strained ethylene-propylene-diene monomer (EPDM) rubber using molecular dynamics simulations of cross-linked and uncross-linked EPDM models at three pressurization levels (20, 40, 80 MPa) relevant to the hydrogen infrastructure. We report the diffusion coefficients of hydrogen gas as a function of nominal strain and describe the hydrogen accessible free volume in strained configurations that determine the magnitude and behavior of hydrogen mobility. This work is valuable as input to higher length scale diffusion-deformation models that are dependent on values of principle strain to predict damage as well as experimental efforts that seek to identify changes in structural features due to hydrogen exposure.

Entrapment of Volatile Organic Compounds in MOF UiO-66: An ab initio molecular dynamics study

Brianne Boyd[1], Deep Choudhuri[1], N. Scott Bobbitt[2]
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Speaker: Brianne Boyd

Volatile organic compounds (VOC) are produced by various pathogenic pathways due to the interaction between viruses and the body’s immune system. Interestingly, such VOCs can be trapped within the pores of hybrid organic-inorganic Metal-Organic-Framework (MOF) - a relatively new category of material. Here, we have examined the entrapment mechanism of 2-butanone VOC within the octahedral pores of Zr-based UiO-66 MOF by employing Ab initio molecular dynamics (AIMD). Simulations were performed using NPT ensemble, and the entrapment process was characterized by computing VOC/UiO-66 interaction energies and local intermolecular bonding at 300K and 500K. We probed this interaction for different loadings of 2-butanone with and without water molecules by placing them within pristine and defective UiO-66 frameworks. Our results indicate that 2-butanone molecules interacted favorably with UiO-66 in the absence of moisture, which was aided by the diffusion of the VOC throughout the interstitial sites of the MOF structure.

How to Feed AI: Creating a Cu-Ag Alloy Nanocrystalline Thin Films Library for Materials Informatics

Kyle Dorman[1], Manish Jain[1], Sadhvikas Addamane[1], Catherine Sobczak[1], Nathan Bianco[1], Saaketh Desai[1], Remi Dingreville[1], David Adams[1]
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Speasker: Kyle Dorman

Modern accelerated materials science development makes extensive use of machine learning and neural networks to analyze large, well-curated datasets. For investigation of novel material systems, such as the recently discovered grain-boundary segregation stabilization of nanocrystalline bimetallic thin films, this requires extensive work from experimentalists to generate a useful, relevant thin film library to which data science can be applied. In this study, a compositional and deposition process parameter survey of Cu-Ag thin films was performed both in search of improved metal contacts and as a means to enable AI-driven materials discovery. Using the combinatorial deposition techniques of [McGinn et al., ACS Comb. Sci. 2019] and iterating on the workflow of [Adams et al., JVST 2024] in the excellent but expensive Pt-Au thermally stable nanocrystalline system, 896 thin films were deposited using 8 pulsed DC magnetron sputtering depositions. Then 7 modalities were measured, supplemented by selected TEM sections to further understanding of the microstructure, producing a thin films material library for both concurrent and future use in materials science research.

CO_2 Adsorption at Metal Nodes of Mg-MOF-74 : An Ab Initio Molecular Dynamics Study

Gabriel Beltran[1], Deep Choudhuri[1]
[1]Department of Materials and Metallurgical Engineering, New Mexico Tech, Socorro, NM

Speaker: Gabriel Beltran

Metal–Organic Frameworks (MOFs) are well-known for adsorbing foreign gaseous molecules like CO_2, SO_2, and volatile organic compounds. Here, we have investigated the adsorption mechanisms of carbon dioxide inside a magnesium-based MOF (Mg-MOF-74) by utilizing ab initio molecular dynamics. These simulations were performed using an isobaric-isothermal (NPT) ensemble, where CO_2-Mg-MOF-74 composite structures were subjected to a temperature of 300K and near-ambient pressure. Results were analyzed by computing interaction energies and probing the bond-formation mechanism as a function of CO_2 concentration, for loading up to 10 molecules of CO_2. We found that interaction energies monotonically decreased with increasing CO_2 content between the gaseous molecules and node sites of our framework. This energy reduction was facilitated via mono dentate Mg-O-(CO) coordinate bond formation.

The effect of laser remelting on the microstructure and chemistry of additively manufactured MoNbTaTi RHEA

Erin Barrick[1], Andrew Kustas[1], Christian Harris[1], Levi Van Bastian[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Erin Barrick

****INVITED SPEAKER****

Refractory high entropy alloys (RHEAs) are emerging materials that have attracted attention for exceptional properties, such as high melting temperatures, retention of high-strength at elevated temperature, and resistance to degradation in harsh environments. Additive manufacturing (AM) is an appealing processing route for refractory alloys which have historically been challenging to fabricate via conventional manufacturing routes. In this study, blown powder laser beam directed energy deposition (L-DED) was used to additively manufacture compact metallurgical samples of equiatomic MoNbTaTi starting from elemental powder feedstock. As a result of the challenges of fully melting the elemental constituents and achieving homogeneous chemistry, a laser remelting step was integrated after each deposition layer. Development of satisfactory remelting parameters involved variation of the laser power. Novel metallographic etching techniques were developed to enable observation and measurement of individual melt tracks to understand the effects of processing on print quality and microstructure. Scanning electron microscopy including electron backscattered diffraction (SEM/EBSD) was used to observe microstructural changes across different processing parameters and to understand cracking, likely occurring from interstitial element impurities. Unique crystallographic textures were observed resultant of the remelting conditions. The as-built composition of the builds was determined using wavelength dispersive spectroscopy (WDS) and analytical chemistry techniques. Utilizing elemental feedstocks with widely varying thermophysical properties results in challenges with achieving target chemistries. Printing strategies to overcome such challenges will be discussed. The techniques developed in this work can be adapted to other RHEAs and refractory alloys to enable successful printing with elemental powders and have important implications for full-scale adaptation of these alloys with regards to compositional control and impurity element concentrations.

Enabling Ductile Failure Prediction in Additively Manufactured Metals via 3D Characterization

Paul Chao[1], Ivana Hernandez[2], Thomas Cisneros[3], Suhanna Bamzai[4], Chad Hovey[1], Brian Phung[5], Ashley Spear[5], John Emery[1], Andrew Polonsky[1]
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[2]University of Texas El Paso
[3]New Mexico State University
[4]Georgia Institute of Technology
[5]University of Utah

Speaker: Paul Chao

Our multidisciplinary team devised a robust set of experiments to improve failure prediction in 3D printed components, addressing challenges in ensuring their structural integrity and reliability. Traditional manufacturing methods produce materials with predictable properties, but 3D printing can introduce additional complexities with anisotropic mechanical response and inherent defects. These defects can serve as initiation sites for failure, leading to premature fracture or fatigue that is difficult to predict. This research employs digital twin technology - a virtual representation of a physical object or system - to enable real-time monitoring, analysis, and optimization of components throughout their lifecycle. Here we present the analysis of over two dozen 316L stainless steel tensile specimens made with varying Additive Manufacturing (AM) processing parameters. By quantifying defects such as porosity before and after tensile testing with x-ray computed tomography (CT), we predict failure locations in these specimens through two computational methods: direct numerical simulations (DNS) using Finite Element Modeling (FEM), and a lightweight approach based on void descriptors. Comparisons between these modeling approaches and ground-truth experimental data provide a path forward for improving failure prediction models in AM parts. The suite of user-friendly tools and pipelines developed for these analyses to enable high-throughput 3D analysis will also be presented.

Custom cathode optimization for electropolishing additively manufactured 316L stainless steel

SMichael Melia[1], Mary Louise Gucik[1], Jason Taylor[1]
[1]Sandia National Laboratory, Albuquerque, NM

Speaker: Kasandra Escarcega Herrera

Laser powder bed fusion (LPBF) has become increasingly popular for its ability to create complex geometries. However, LPBF creates tortuous surfaces that may degrade overall performance. Consequently, post-processing is often needed for LPBF parts through techniques such as electropolishing (EP). Utilizing COMSOL, this project aims to enhance EP of a LPBF 316L T-shaped part in a polyethylene glycol/NaCl based electrolyte by optimizing the cathodes to smooth the T-shaped surface more efficiently. First, different electrode spacings were experimentally compared using a 316L flat lattice cathode. Next, cylindrical and conformal cathodes of increasing sizes were evaluated. Based on those results, a cathode was then optimized using COMSOL to polish an anode selectively and uniformly. Roughness measurements and optical images were acquired and compared before and after polishing to quantify EP efficacy.

Structural and failure mechanisms - Automated Calibration of Displacement Sensors

Kim Haulenbeek[1]; Ernest Miramontes-Carrera[1], Mark Foster[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Kim Haulenbeek

Calibrating displacement sensors can be a tedious process requiring up to an hour per sensor. Current methods require manual entry of each data point, inviting errors into the process. A new process has been developed that correlates output from a calibrated micrometer head (used as the standard) with the signal from the displacement sensor being calibrated. Code has been generated to define the calibration points and to calculate the error. Further, the motion of the micrometer head has been motorized, thereby eliminating the need for the operator to manually control the process. These developments have led to calibration time being reduced from 30–60 minutes per sensor to 5–10 minutes per sensor.

Improved Kovar Quantification Using LA-ICP-MS

Pamela Coleman[1], Jada Beltran[1]
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Speaker: Pamela Coleman

Kovar is a material used in the brazing of ceramic metal joints. In an effort to learn more about the composition of Kovar received from the manufacturer, it was digested in an acid matrix and analyzed using Inductively Coupled Plasma Optical Emissions Spectroscopy (ICP-OES) for major constituents and Inductively Coupled Plasma Mass Spectroscopy (ICP-MS) for minor impurities. Using this technique to analyze Kovar brought about many challenges such as lengthy digestion time, multiple serial dilutions, and the use of hazardous acids. Laser Ablation Inductively Coupled Plasma Mass Spectroscopy (LA-ICP-MS) was identified as a new and improved method to quantify the major constituents and minor impurities in Kovar. This innovative technique uses a high-irradiance laser to remove particles from the surface of the Kovar. Helium is used as the carrier gas to introduce the particles into the ICP-MS for ionization and detection. Using LA-ICP-MS has many advantages such as a considerable reduction in analysis time, spatial resolution capabilities, and reduced chemical hazards. The use of a NIST Kovar Certified Reference Standard provides accurate, precise, and repeatable quantitative results. In conclusion, quantification of Kovar using LA-ICP-MS has improved the quality of the results, reduced the amount of time needed for analysis, eliminated the need for hazardous chemicals, and added spatial resolution capabilities.

Characterization of oxidation in tantalum and cracking susceptibility at high temperatures using AES

Mila Nhu Lam[1], Melissa Meyerson[1], Chris Finfrock[1], Zahra Ghanbari[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Mila Nhu Lam

Tantalum is broadly used due to its superior corrosion and temperature resistance, workability, and ductility. Yet, oxygen exposure at high temperatures causes cracking in Ta and Ta alloys, resulting in mechanical failure. However, the mechanisms of oxidation and cracking are not well understood. Here, Auger electron spectroscopy (AES) is performed to characterize local oxidation behavior of tantalum to elucidate fundamental mechanisms of oxygen-based aging and damage. AES is a powerful quantitative technique for chemical surface analysis with high spatial resolution (<10nm lateral/depth) enabling the selective removal of the thin native surface oxide and quantification of local oxygen content. AES is conducted on Ta-10W at various temperatures along with complementary X-ray photoelectron spectroscopy (XPS) to understand specific oxidation states. These results improve understanding of the relationship between cracking susceptibility and oxygen content during accelerated thermal aging.

Effect of Dry Electropolishing on Electron Backscatter Diffraction of Dissimilar Titanium Welds

Landon Schnebly[1], Jessica Buckner[1], Rachel Callaway[1]
[1]Sandia National Laboratories, Albuquerque, NM

Speaker: Landon Schnebly

Electron Backscatter Diffraction (EBSD) was used to map the microstructure and phase distribution of titanium electron beam welds. The titanium welds were made of wrought Ti-6Al-4V welded to additively manufactured (AM) Titan 23 alloy. Titanium alloys can be difficult to index with EBSD, and these dissimilar welds added new challenges, given the variable hardness of phases and alloying dependent on weld or base metal location. Preliminary results following mechanical polishing showed low quality EBSD patterns in select areas of the weld, likely due to surface relief. Meanwhile, sample preparation via dry electropolishing has resulted in higher quality EBSD patterns due to a more even finish. Dry electropolishing uses electrolyte beads to strip extruding material consistently across all features despite differing hardness, multiple phases, and varying microstructures. The EBSD patterns measured after dry electropolishing had greater band contrast allowing for higher map hit rates. Dry electropolishing can therefore be considered as an alternative method for preparing complex titanium samples for EBSD.

Poster Abstracts

(P-U1)

Evaluating the Role of Surface Contamination in Preventing DLC Delamination

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Diamond-like carbon (DLC) films are known for their extreme wear resistance, high hardness, excellent coefficient of friction, and low sensitivity to humidity. This makes DLC coatings ideal for critical tribological applications with high contact pressure in non-hermetic environments for high reliability applications. These excellent material properties stem from its mixture of sp2C and sp3C bonds, which impart the coatings with diamond-like hardness and wear resistance while maintaining the lubricity of graphite. However, problems arise in the fabrication of these films as significant residual stress builds as the films are deposited. This extreme film stress, often higher than 1 GPa at the coating interface, will cause delamination if proper steps are not taken to prepare the substrates surface for film adhesion. In this study, the effects of surface contamination are interrogated. DLC films were deposited on samples of various contamination levels. The contamination was controlled by dosing varying concentrations of detergent (Dirl-Lum 603) from solutions of 4.7wt.%to 1.6x 10-5wt.%in water. Additional samples contaminated with 2-propanol and acetone were also studied. A standard plasma enhanced chemical vapor deposition DLC coating was used to create a-C:H films. Optical microscopy was used to determine a sensitivity threshold of the coated film to an arial density of detergent. Optimal cleaning solutions and coating modifications are demonstrated.

(P-U2)

Dissimilar metal joining of Ti-6Al-4V and 304L Stainless Steel

Ethan Hopwood[1], Brett Roper[1], Austin Pisani[1], Jack Herrmann[1], Erin Barrick[1]
[1]Sandia National Laboratories, Albuquerque, NM

The joining of Ti-6Al-4V and 304L stainless steel through the use of a suitable interlayer shows potential for design flexibility by avoiding the detrimental intermetallic phases that form from direct welding. Different interlayer application methods were investigated, including cold sprayed 304L onto a Ti-6Al-4V substrate, a directed energy deposition (DED) vanadium layer deposited onto a Ti-6Al-4V substrate, and a vanadium sheet interlayer. Vanadium was chosen for its high metallurgical compatibility with both Ti-6Al-4V and 304L stainless steel. Laser welds were made in continuous wave, beam oscillation (wobble), and pulsed modes, with laser powers that ranged from 375W to 850W. Transverse cross sections of the welds were metallographically prepared from all three methods and were analyzed to understand microstructure and weld defects using optical and scanning electron microscopes. Welds between the cold sprayed 304L and the 304L parent material exhibited favorable qualities and had minimal porosity. The DED vanadium and 304L welds had more porosity relative to both other sets. This is likely from higher porosity in the DED vanadium layer initially. The vanadium sheet welds showed the least amount of porosity with the Ti/V joint containing more than the 304L/V. Interweld cracking was minimal in all the joining methods but was seen in the pulse and wobble welds. Extensive interlayer cracking was seen in both the cold sprayed 304L and DED vanadium layers, likely due to unoptimized interlayer deposition parameters. Once optimized all three methods show promising results for joining Ti-6Al-4V and 304L stainless steel while avoiding the formation of brittle intermetallic phases.

(P-U3)

Transition Metal-doped Hydroxyapatite with natural medicinal compounds for orthopedic applications

Gwenevere Gatto[1], Joel Pilli[1], Nusrat Yeasmin[1], Arjak Bhattacharjee[1]
[1]New Mexico Tech

Hydroxyapatite (HA)-based bioceramic materials are used for musculoskeletal reconstruction, due to their compositional similarities to human bone tissues. However, this often leads to graft failure due to infections. Post-surgical bacterial infections on hydroxyapatite grafts are known as osteomyelitis which leads to more painful and expensive surgeries to fix the issue. This research aims to dope hydroxyapatite with transition metal oxides that are expected to incorporate antibacterial properties. The phase identification studies show no adverse effect as a result of doping. The fabricated grafts are being used as an alternate drug delivery vehicle with various plant-derived natural medicinal compounds. Careful optimization of the compositions does not show any adverse effect on the cytocompatibility with fibroblast cells. These novel scaffolds could be used for various orthopedic and dental applications.

(P-U4)

Evaluation of Material Properties for Flexible Coatings

Mariah Strauss[1] and Corey Parada[1]
[1]Sandia National Laboratories

Polymer-derived materials are often categorized as either thermoplastic or thermoset materials. Upon curing, thermoset materials create irreversible chemical bonds, resulting in structurally robust materials that find use in applications ranging from high-performance composites, specialized fibers, and commercial rubbers and coatings. For coating materials specifically, selection of starting materials and their stoichiometric ratios are two driving factors that must be considered when formulating these materials, alongside other variables such as curing temperature and processing time. In this study, different ratios and combinations of common epoxies, curing agents, and flexibilizers were used to find a material with desirable properties. Analysis of several material properties was conducted including glass transition temperature of each cured material which ensures high flexibility at a wide range of temperatures.

(P-U5)

The Influence of Borate Additives on Cathode Electrolyte Interphase Stability for Li-ion Batteries

Arianna N. Serrano[1] and Nathan T. Hahn[1]
[1]Sandia National Laboratories

Lithium-ion batteries are a critical technology for vehicle electrification, and improvements in battery performance, cost, and lifetime are important for maximizing their effectiveness. Among the positive electrode (cathode) materials for Li-ion, the layered oxide $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) and the disordered rock salt oxy-fluoride $Li_{1.2}Mn_{0.6}Ti_{0.2}O_{1.8}F_{0.2}$ (LMTF) are emerging as promising candidates. This promise is due to their high energy density and the reduced or eliminated cobalt content leading to lower costs and increased sustainability in comparison to more traditional cathode materials. However, current issues with cycling stability, particularly poor capacity retention at high cycling voltages due to an unstable cathode-electrolyte interface (CEI), are preventing these materials from broad adoption. To address this, various electrolyte additives are employed to stabilize the CEI and improve the overall cyclability. These additives may mitigate electrolyte decomposition and transition metal dissolution by forming a protective CEI through preferential oxidation or by scavenging fluoride byproducts, mainly HF. A series of borate additives were evaluated within a standard Li-ion electrolyte to understand their influence on CEI formation and cell cycling performance for the two cathode exemplars mentioned above. Through electrochemical testing and surface characterization it was concluded that inorganic borates showed better CEI stabilization in half cells (cycled vs. Li metal) for NMC811. However, for LMTF, poor performance was observed regardless of additive due to its unique surface chemistry. These findings assist in the understanding and design of improved electrolytes for next generation Li-ion batteries.

(P-U6)

UNM's Hot Cell Facility for Remote Mechanical Testing: Cryogenic and High-Temperature Capabilities

Louis Sanchez[1], Jared Justice[1], Osman Anderoglu[1], Stuart Maloy[2]
[1] University of New Mexico
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Advanced nuclear reactors offer promise for sustainable energy development capable of meeting the world’s growing energy need. These advanced reactor technologies require development of high-performance materials that can operate at higher temperatures under high dose neutron irradiation while in contact with corrosive coolants. Establishing microstructure-mechanical property relations is one of the fundamental components of research and development of high-performance alloys. Therefore, the newly established remote control hot cell mechanical testing facility at the University of New Mexico capable of handling radioactive specimens at temperatures up to 900°C is a unique capability that will play an important role in advanced reactor development. Furthermore, the facility can also perform cryogenic temperature testing which is important for future experiments involving fusion reactors as well as transportation of spent fuel. This presentation will detail the set-up, specimen holder design, recent test results of various commercial alloys considered for advanced reactors, as well as future plans improving the hot cell’s capabilities.

(P-U7)

Metal-Organic Frameworks for Selective Adsorption of Rare-Earth Elements in Aqueous Environments

Caith McKeown[1], Dorina Sava-Gallis[1], Eric Sikma[1]
[1]Sandia National Laboratories

Rare-earth elements (REEs) are used in manufacturing computer chips and other modern technologies. REEs are largely imported from outside of the United States, but increased needs in these industries have created a high demand for these materials and necessitate a new energy efficient method of sourcing REEs. One such way is the recovery of REEs from wastewater, which provides a recyclable and domestic method of obtaining REEs. Metal-organic frameworks (MOFs) serve as a promising platform for REE capture owing to their high porosity and high degree of tunability of pore sizes, shapes, and chemical compositions to infer selectivity towards desired REEs. In this we work we report the synthesis, characterization, and testing of a family of MOFs, UiO-66-X, functionalized with halogen groups (X = -F, -Cl, -Br, -I). This systematic platform allows us to study the effect of organic linker functionality on the adsorptive selectivity and/or adsorptive capacity towards REEs in aqueous environments. A suite of techniques was used to characterize these systems. Phase purity and crystallinity was confirmed via powder X-ray diffraction (PXRD) studies, thermal stability was examined via thermogravimetric (TGA) analyses, and porous qualities were probed by measuring the N_2 adsorption isotherms at 77K. Competitive studies for selective REE are ongoing.

(P-U8)

Static and Dynamic Thermomechanical Properties of Phase-Separated Epoxies with Tuned Microstructures

Francesca M. C'deBaca[1], Brad H. Jones[1], Erin J. Nissen, Angela Ku[1], Jessica W. Kopatz[1], Nha Uyen Huynh[1], Samuel C. Leguizamon[1]
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Epoxies are prevalent in a variety of technical industries due to their physical and chemical stability, tensile and compressive strength, as well as their adhesive capabilities. However, both research and industry alike demand new materials that build upon these favorable properties. While processes exist to increase efficacy and efficiency in their respective fields, one method presents itself as an ideal solution: the construction of heterogenous epoxies, which result in properties that surpass those of more common homogenous epoxies. In this work, we focus on the use of phase-separated epoxy networks as encapsulants for microelectronic devices by conducting a wide range of thermomechanical testing to observe their static and dynamic properties. The epoxies consist of hard and soft domains with phase-separated length scales systematically tuned from macro-scale (µm+) to nano-scale (ca. 10 nm). The glass transition (T_g) profile of the macro-phase epoxies exhibit two separate relaxations - indicative of individual glass transitions of the phases, whereas the T_g of the nano-phase materials exhibit a broad curve, indicating a complex composition. In compression at both quasi-static and dynamic rates, the nano-phase samples generated greater modulus and strength than the macro-phase samples. The thermal expansion behaviors of these epoxies are driven by the complex glass transitions, where in particular the nano-phase epoxies appear to have lower residual stress accumulation. In sum, we can assert that heterogenous epoxies, particularly nano-phase separated, will make for highly resilient encapsulants due to their high modulus and strength, and their characteristic low residual stress, without forgoing their capacity to support loads.

(P-U9)

Predicting Electrochemical Responses using Machine Learning

Matthew Roop[1,2], David Montes de Oca Zapiain[2], Aditya Venkatraman[2], Sam Moran[2], Rebecca Schaller[2], and Ryan Katona[2]
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The electrochemical response of metals can be ascertained through various methods. Potentiodynamic polarizations provide electrochemical behavior of a metal in an electrolyte solution. Polarization curves are generated through physical experiments which can be costly. Machine Learning (ML) was used to predict polarization curves from metal and electrolyte properties without conducting physical experiments, saving time and resources. However, there is no suitable repositories for holding polarization curves properly that is easily accessible to ML. To solve this issue, a database has been constructed using python specifically for storing electrochemical data and extracted properties. This database, however, is sparse. The database uses ML to identify experimental conditions so that minimal scans need to be obtained through physical experiments to produce a satisfactory model able to predict electrochemical materials' performance.

(P-U10)

Quantifying Oxidation of Hafnium, Niobium, Tantalum, and Zirconium High Entropy Alloy

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Newer generation heat engines and exchangers – such as hydrogen internal combustion engines – achieve high efficiencies because of the high temperatures that are reached inside of the combustion chambers. These temperatures can reach as high as 1500 °C, which many current steels and alloys cannot withstand. As temperatures and efficiencies continue to rise, new materials are needed to be developed that are able to withstand these high temperatures. High entropy alloys (HEAs) are a class of materials composed of 4 or more elements mixed in nearly equiatomic compositions and have shown the potential for improved material performance in high temperature, corrosive, and irradiation environments. This work explores the oxidation and irradiation performance of a HfNbTaZr. Isochronal annealing at 600, 700, 800, and 900 °C coupled with mass change measurements enable calculation of the oxide growth rate, while in-situ Thermogravimetric Analysis (TGA) and in-situ X-ray Diffraction (XRD) up to 900 °C decipher the real-time phase and oxide growth changes. Post-exposure analysis with XRD and SEM offer information on the development of new phases and the spatial distribution of oxide formation. XRD analysis provided valuable information about the likelihood of each element oxidizing, with Ta and Zr being much more likely to oxidize as compared to their Hf and Nb counterparts. This was in contrast to the in-situ SEM annealing experiments, highlighting the differences between testing techniques. Finally, initial results on the irradiation stability of the HfNbTaZr HEA under 2.8 MeV Au ion irradiation offers insights on the performance of this HEA composition in multiple extreme environment conditions. This work can inform future alloy design to develop optimized HEAs and materials to better withstand higher temperatures, which is a key cornerstone to next generation Carnot heat engines – and the next step towards a zero-emission world.

(P-U11)

Electrolytic etch uniformity of 304L stainless steel

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304L stainless steel is crucial in various industries due to its excellent corrosion resistance, balance of strength and ductility, enhanced weldability, and reduced risk of intergranular corrosion. Effective preparation and etching procedures must be developed to reveal microstructural constituents. Electrolytic etching of 304L stainless steel involves using an electrolyte solution and electrical current to selectively remove material from the surface. This reveals grain boundaries, phases, and other microstructural features for metallographic examination. A primary issue with current 304L stainless steel etching techniques is the inability to achieve a uniform etch across the entire surface of larger (>2 inch) samples. Variations in etch uniformity can result in a failure to reveal true microstructural features. This study focuses on cathode-anode geometry, sample placement within the electrolytic cell, electrolyte selection, voltage applied and etch duration to optimize the etch response of 304L. A wide variety of stainless-steel cathodes will be tested ranging from large sheets to small rods. Anode placement will be tested by connecting the stainless-steel anode to various regions on the sample. The electrolytes used in this study are ASTM 219 (60:40 HNO_3 & DI H_2O) and Oxalic etch (10g $C_2H_2O_4$ & 100mL DI H_2O). All tests are conducted on 25mm x 40mm samples of 304L mounted in 2” epoxy mounts. The results of this parametric study will uncover promising and practical electro-chemical etching combinations, enabling our metallography lab to confidently characterize 304L microstructures pertinent to Sandia’s laser welding and microstructure development research portfolios.

(P-U12)
Computational Phase Diagram of Al-Si Binary Alloy Using Thermodynamic Integration Method

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Aluminum-Magnesium (Al-Mg) alloys are integral to the automotive and shipping sectors due to their high strength-to-weight ratio, stiffness, and corrosion resistance. However, the additive manufacturing of these alloys faces challenges primarily due to defects that occur at high solidification rates. One approach to mitigating these defects is by promoting equiaxed grain growth over columnar grains during solidification. In this study, we computationally predict two critical interfacial properties—interfacial energy and its anisotropy—in an Al-Mg system using molecular dynamics simulations. The first phase of our research focuses on calculating an accurate binary phase diagram for the Al-Mg system through the Gibbs Thermodynamic Integration method. Our results are then compared with the existing binary phase diagram and data from the Monte Carlo-based atom swap technique. This computational framework not only provides insights into Al-Mg alloy behavior but also lays the groundwork for extending the analysis to ternary systems.

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(P-U13)

Atomistic Simulations of "Forever Chemicals"

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Per- and polyfluoroalkyl substances (PFAS), a class of highly fluorinated hydrocarbons, pose global contamination and pollution concerns due to both their toxicity and their potential to increase risks of reproductive disorders, endocrine disruption, and cancer. The resistance of such substances to degradation in the environment has earned them the title of “forever chemicals.” Two of the most abundant PFAS species, Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS), have been associated with tens of thousands of deaths annually. Despite extensive recent efforts, analysis of the molecular-level behavior of PFOA and PFOS has remained elusive.

To address this knowledge gap, we conduct extensive investigation of the properties of PFOA and PFOS through first-principles electronic structure and molecular mechanics calculations. Utilizing both classical Molecular Dynamics (MD) and quantum Density Functional Theory (DFT) techniques, we perform structural optimization of PFOA and PFOS molecules in simulation cells; such structures are utilized to characterize time-evolution of molecular systems. We also study chemical properties of PFOA and PFOS when placed in larger systems, such as diffusion in aqueous environments and hydrophobicity. Our MD and DFT-MD results align closely with experimental results and contribute the first detailed atomic-level studies of PFAS substances. Moreover, we discover atomic-scale reductive defluorination of PFOA catalyzed by Cobalt-containing Vitamin B12 complexes, furthering our understanding of PFOA degradation mechanisms. Thus, our study provides a molecular-level basis for mitigating the toxic effects of PFAS substances.

(P-U14)

A Science-based Approach for Agile Injection Molded Parts: 3D Printed Plastic Molds

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Injection molding is traditionally reserved for high-volume production due to the significant costs and lead times associated with fabricating metal tooling. The substantial initial investment is justified by the efficiency of injection molding in producing large volumes of parts. Until recently, low-cost and fast turnaround additively manufactured (AM) tooling was not a viable option for injection molding due to limitations in material selection and the resolution of printed components. In this study, we investigated the deformation of AM plastic molds under the high temperatures and pressures encountered during the plastic injection process. We employed advanced modeling and simulation techniques to analyze heat flow and plastic warpage, aiming to predict AM mold longevity and optimize mold design by accounting for dimensional changes to ensure the mold meets tight tolerances. An additional advantage of the design flexibility offered by AM technology is the seamless integration of intimate contact sensing capabilities. In this instance, temperature sensors were mounted on AM printed circuit boards that were themselves embedded within the molds, providing critical data for modeling and simulation. This innovative approach facilitates low-volume, cost-effective manufacturing of injected plastic components, and lays the foundation for rapid prototyping using a technology traditionally reserved for mass production.

(P-U15)

'DECIEDD with CARE' - Building an Autonomous Ecosystem for the Discovery and Optimization of Metal Nanoparticle Inks

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The end-to-end design and manufacturing of printed circuit boards substrates, a ubiquitous and critical technology in energy storage, communication, and defense systems, is poised to undergo a transformation following developments in additive manufacturing within the last decade. These advancements include droplet-on-demand inkjet printing of conductive inks—suspensions of metallic nanoparticles, graphene, carbon nanotubes, etc.—onto dielectric substrates. Despite extensive research, few printed commercial inks possess the conductivity and robustness desired by high-reliability design agencies. A major contributor to the limited availability of viable inks is the enormous parameter space of processing conditions and material structure, property, and performance criteria that must be balanced during development.

For this reason, Sandia National Laboratories, together with university partners, has engaged in the design and implementation of an autonomous materials discovery platform to efficiently (1) synthesize Cu, Ag, and Au nanoparticles, (2) formulate those nanoparticles into inks, and (3) print those inks to form devices. At each step of the process, characterization data of the structure, properties, and performance is provided to a machine learning algorithm utilizing a self-consistent and scalable/tunable data schema and data management application. Initial campaigns have utilized off-the-shelf machine learning methods to autonomously optimize the size and dispersity of silver nanoparticle via manipulating the stoichiometric ratio of mono-, di- and tri- functionalized carboxylic acid ligands, amongst other variables. Concurrently, development of bespoke solutions such as multifidelity reinforcement learning and scientific machine learning continues to address the challenges of relatively sparse data sets, multimodality and fidelity, and the need identify underlying process-structure-property-performance relationships.

To expedite nanoparticle ink characterization, we are developing a high-throughput, model to characterize the rheology of nanoparticle inks. Printing microelectronics requires specific rheological properties, necessitating an automated process for determining the rheology of these inks. In this study, we introduce novel methods to calculate surface tension and viscosity using image processing with a high-speed camera. Video frames are analyzed in two distinct regimes: the pendant regime for calculating surface tension and the free-falling regime for determining viscosity. Our code employs the Method of Selected Planes, an estimation of the Young-Laplace equations, to estimate surface tension. For viscosity, we track the oscillations of a falling droplet. Preliminary results using water as a sample fluid show that our surface tension model achieves an accuracy within 15%. This approach promises to significantly enhance the efficiency of microelectronic ink development.

(P-G1)

Enhanced Optical Resonances in Transition Metal Dichalcogenide Metasurface

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Transition metal dichalcogenides (TMDs) are a class of materials with the general formula MX_2, including tungsten disulfide (WS_2) and molybdenum disulfide (MoS_2), as well as their diselenide counterparts. These materials have garnered significant attention due to their intriguing electronic, optical, and mechanical properties. TMD monolayers can be incorporated into designs of devices based on metamaterials and nanostructures with Mie resonance to enhance optical response and light-matter interaction. Key research areas include optimizing fabrication techniques to control the size and shape of TMD nanoantennas to achieve desired Mie resonance effects, developing hybrid materials that integrate TMDs with plasmonic nanoparticles or other resonant structures, and creating models to predict and understand the interactions between TMDs and Mie resonances. Recent studies have reported strong coupling between interlayer excitons in WS_2/MoS_2 van der Waals (vdW) heterostructure and cavity-enhanced Mie resonances in individual, where mode splitting in scattering and tunable interlayer excitonic emission are observed. As has been reported, the film quality of TMDs can significantly affect both their electronic properties and exciton coupling. However, it is unclear how the film quality affects the interlayer exciton coupling in vdW heterostructure and Mie-resonant nanoantennas. In our research, we focus on a high-quality WS_2/MoS_2 heterostructure film with a large single crystalline domain grown on Si/SiO_2 wafer substrate (50 nm SiO_2 + 200 nm Si + 375 nm SiO_2 + back Si). We investigate the effects of metasurface parameters in detail on the controlled growth of these heterostructure films, stacking, and pattering. With optimized growth conditions, the heterostructures are then integrated with a dielectric platform to realize effective energy exchanges and Rabi oscillations. Furthermore, we explore expanded heterostructures ($WS_2/MoS_2/WS_2$) combined with cavity-enhanced Mie resonances on the mode splitting in scattering and interlayer excitonic emission. We focus on investigating the Purcell effect, which is a phenomenon occurring when the spontaneous emission rate of an excited emitter (such as an atom or quantum dot) is enhanced by its coupling to a resonant optical cavity. We conduct a theoretical investigation of the spontaneous emission enhancement of a dipole emitter. The WS_2 integrated nanoantennas support localized resonant modes that match the emission wavelength of the dipole emitter, leading to the confinement of an electromagnetic field at the antenna's surface, and an increase in the Purcell factor of dipole emitters located near the antenna. Our analysis is directed at further boosting the Purcell effect by using the WS_2/MoS_2 heterostructure. These results advance the design of TMD heterostructures with various excitonic states and enhanced Mie resonance for highly sensitive sensors or devices with tunable optoelectronic properties.

(P-G2)

Scalable Processes for Ultrafiltration Membranes

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Global population increase this century will result in increased demand for potable water. This will occur simultaneously with a decreasing supply due to the effects of climate change. This tenuous situation requires more environmentally friendly methods of water filtration. One such method is membrane distillation. These membranes can be created using ultrafiltration membranes modified to increase hydrophobicity. The traditional method of production of these membranes involves a process called nonsolvent-induced phase separation which is then modified to increase hydrophobicity. This process is characterized by the use of large quantities of organic solvents which are ecologically damaging. The modification process then decreases flux and makes the process difficult to scale. Templating is a method of production which forgoes the use of solvents. It offers the advantage of in-situ modification of the membrane through self-organization kinetics when an amphiphilic block copolymer is used as the surfactant. This process can be scaled without a reduction in flux rate while also reducing the tendency for phase separation, a common issue with the self-organizing templating method. This work is dedicated to determining a less ecologically damaging scalable method of production for ultrafiltration membranes with applications in membrane distillation. Casting and curing procedures were optimized for scaling. Different support substrates and protective intermediate layers were explored. This work was analyzed using scanning electron microscopy, contact surface angle goniometry, and flux rate testing. A scalable method for production of ultrafiltration membranes was determined with the ability to produce long rolled sheets with minimal intensive intermediate steps. Flux results indicated a significant improvement in rate with an increase in flux from 38.5 mL/hr·cm2 @ 1.36 atm at the small scale, to 70.8 mL/hr·cm2 @ 1.36 atm with the scalable method of production.

(P-G3)

Zirconia-hydroxyapatite composite with curcumin as a drug to prevent oral infection.

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Periodontitis causes loss of tooth and damage of periodontal tissues. According to WHO about 19% of total adults in the worldwide are affected by periodontal disease. Treatment of periodontitis is challenging because of bacterial growth after the treatment. Additionally, higher cost of dental treatment is a significant burden to the patients. Bioactive materials are needed to regenerate healthy tissue. The objective of this study is to use active biomaterial Hydroxyapatite which has chemical properties like bone. Hydroxyapatite is brittle in nature and lacking mechanical properties. To improve its mechanical properties, we selected zirconia which has low reactivity, inert nature, and good mechanical and optical properties. However, Zirconia with Hydroxyapatite will produce some unnecessary reactive products. Hence, our strategy is to use transition metal-doped zirconia that can further improve its mechanical properties. Previous studies have reported that bacterial infection and biofilm growth over the dental implant surface may lead to implant failure. Our strategy is to use an alternative antibacterial compound, curcumin from turmeric extract to address this problem. Curcumin is antibacterial, antioxidant and anti-inflammatory in nature. In this study, we will use bioactive material curcumin as a natural medicinal compound to prevent dental oral infection.

(P-G4)

Retarding Field Energy Analyzer Based Analysis of DC Sputtered Ultra High Performance MoS2

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Sputter deposited molybdenum disulfide (MoS_2) dry lubricants have a long-standing history in the aerospace industry because of their ultra-low friction and high performance in vacuum. While these films have shown promise, achieving consistent films has been a persistent challenge. The industry is often plagued with low-density and high porosity films which have worse oxidation resistance and reduced wear life. To address these issues, many have resorted to doping MoS_2 coatings with various metals (Ni, Ti, Au) and nonmetals (PbO, Sb_2O_3, C) to improve density and repeatability. Unfortunately, this approach often results increases in initial friction, particularly after aging. In this study, we utilize a retarding field energy analyzer (RFEA) to characterize the deposition flux in situ. This state-of-the-art tool allows us to study the plasma characteristics of depositions that resulted in differing material properties (crystallinity, hardness, modulus, and stoichiometry) and tribological performance (friction, run-in, and wear rate). The relationships in this study provide a potential guide for future developers exploring MoS_2's complex design space, thereby accelerating the optimization process. The resulting undoped films are near bulk density with low initial friction before and after aging.

(P-G5)

Digital Image Correlation to Quantify Strain Transfer in Organ-On-A-Chip Models

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Introduction

Traumatic brain injuries (TBIs) can result in life-altering complications and are present in military and civilian populations. TBI damage mechanisms are not fully realized due to minimal access to the human head during TBIs. The Anthropomorphic Neurologic Gyrencephalic Unified Standard (ANGUS), a validated full-scale head model, is used to observe deformation and cavitation under impact scenarios. ANGUS lacks biological components to identify injury thresholds therefore, a cerebral organ-on-a-chip (COCh) model consisting of cerebral organoids embedded in polyacrylamide (PAA) hydrogel chips was fabricated. Three designs were fabricated to investigate what strain organoids experience when embedded in different configurations. Cellular injury is often determined with strain and strain rate, therefore understanding how strain transfers from the chip to the organoid makes it possible to link biological damage to different strain levels experienced by the organoid.

Methods

PAA was poured into polydimethylsiloxane molds to make three hydrogel chips. Microwell molds had organoids in direct contact with PAA and surrounded by Matrigel, an extracellular matrix gel acting as a feeder layer for cells. Cylinders molds encased the organoid in a Matrigel plug within the chip. Lastly, surface molds had organoids in direct contact with PAA near the gel surface for imaging and were then encapsulated in Matrigel. Organoids grew in the gel for 14 days and were then sheared in a custom shear device from Suhas, V., 2021. The chips were speckled and compressed by 10% between a dynamic and static plate and deformed at 30, 50, 70, and 100 Hz at 0.5 and 2 mm of displacement. DIC analysis was then performed with a subset of ~0.3 mm, step size of ~0.1 mm, and strain window of ~0.07 mm.

Results

Chips deformed at 70 Hz & 2 mm of displacement in gels with and without embedded organoids experienced up to 20% strain on the surface. However, microwell molds experienced more than 21% strain. In cylinder chips, the organoid only experienced approximately 8% strain while the surrounding Matrigel displayed greater than 35% strain occurring at the Matrigel-organoid interface.

Discussion

Performing DIC on shear deformation allows for observation of strain experienced by COCh. Cylinder molds with organoids encapsulated in Matrigel experienced strain likely incapable of causing damage whereas in microwell molds they experienced a higher level of strain. This is due to the softer Matrigel material absorbing the deformation limiting strain experienced by the encapsulated organoid, whereas if grown into the PAA chip it experiences strains like that of the chip. Therefore, growing organoids in contact with PAA produces strain capable of causing damage whereas being encapsulated does not. By employing ANGUS with COCh this collaboration aims to understand TBI injury thresholds to limit TBIs by informing equipment design and training policies in sport and military populations.

(P-G6)

Radioisotope Evaporation in Molten Lead for LFR Source Term

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Lead fast reactors are a promising nuclear technology with several advantages over existing light water reactors including fuel economy, safety, and proliferation resistance. Significant progress has been made toward the conceptualization of lead- and sodium-cooled fast reactors. Molten lead is an excellent coolant for advanced fast reactors due to its attractive thermal and neutronic properties. The high boiling point of lead provides a wide margin of safety and enables high temperature operation, and thus higher efficiency. The low vapor pressure of lead means the primary coolant loop of a lead fast reactor does not need to be pressurized, and lead is chemically inert in the presence of other plant fluids. There are still uncertainties regarding the mechanistic source term evaluations of liquid lead cooled fast reactors. The goal of this project is to investigate the effects of fission product interaction with liquid lead to evaluate the mechanistic source term of the lead fast reactor, develop a test methodology for liquid metal source term calculations, and establish a basis for comparison of fission product retention between lead and sodium. A 316 stainless steel test chamber with resistive heating and ceramic fiber insulation was built. Lead, stored in a melt tank was purified and transferred to the test chamber, where fission products were introduced. A rotary feedthrough was used to crush an ampoule containing cesium or iodine inside the lead. The top of the chamber was cooled to below 40°C with a heat exchanger, and stainless steel plates were attached to the cool surface to observe adsorption. These plates were weighed before and after each trial. First, pure lead was tested in the chamber at 550, 600, 650, and 700°C. Subsequently, trials were conducted with 5g of cesium at 550, 600, and 650°C, and then with 5g of iodine at 550, 600, and 650°C. The rate of fission product evaporation was measured. In each trial the amount of mass deposited on the plates was significantly less than the amount introduced. This would indicate that a significant portion of the Cs and I was retained by the lead coolant, which is consistent with earlier solubility modeling in ICP-MS. In a lead cooled fast reactor, this could mean fission products released from fuel pin ruptures during accident conditions would be retained to a large degree by the molten lead, and not escape the containment structure.

(P-T1)

Determining the radiation response of aging COTS parts through Laser Dose-Rate Surveillance testing

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An electronics Laser Dose-Rate Surveillance (LDRS) protocol will be presented to address the effect of aging on the radiation response of Commercial-off-the-shelf (COTS) electronics. The protocol ensures the reliability and longevity of fielded COTS devices by detecting changes in their electrical response because of the combined effect of aging and laser dose rate. It is accomplished through annual dose-rate testing of 'Life-of-Program’ parts and stored in various controlled aging environments. The goal is to detect the onset of small changes in response to radiation applied at a specific dose rate (simulated with laser power) by measuring electrical parametric values. Ongoing testing generates data that can determine the time-dependence of the aging process. Implementation of the protocol has initially focused on six families of COTS-based silicon devices. Examples of the test protocol and resultant data will be presented, though results to date have not clearly revealed any trends in aging or dose-rate effects for the tested COTS devices. This protocol aims to ensure the reliability and longevity of silicon devices by systematically monitoring and analyzing their aging processes.

(P-T2)

Fine Pitch Ball Grid Array (FPBGA) Reliability Evaluation through Thermal/Mechanical Testing

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Fine pitch ball grid arrays (BGAs) allow for higher interconnect density. By decreasing the pitch size, or distance between neighboring solder ball centers, higher computing power can be achieved within a smaller footprint. There has been limited application of fine pitch BGAs within the field of high reliability electronics, and this study seeks to fill the knowledge gap by examining BGA packages with pitches under 1-mm. It details the design and results from a physics-of-failure reliability study for board level ball grid array (BGA) solder interconnects to identify the limiting pitch in terms of interconnect performance/reliability. Thermal cycling of acquired COTS (Commercial Off the Shelf) package types for a predetermined number of cycles and eventually to failure (under electrical monitoring) and analyzes failure modes, failure locations, and failure rates as interconnect pitch values decrease. Analysis includes shear testing, cross-sectioning, and imaging. The outcome(s) of this study will allow future designers and manufacturers to improve cost efficiency, save time/resources, and continue to expand the technical limits of microelectronics research.

(P-T3)

Enzymes Under Confinement: Materials Interactions and Functionality for CO2 Capture and Conversion

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Membranes designed for reactive capture (capture and conversion) of CO_2 are used in industries where large amounts of CO_2 waste is produced. Captured CO_2 can be electrochemically reduced to CO and converted into a value-added product that is industrially important. Typically, these capture membranes consist of an alumina substrate with a nanoporous silica layer. Enzymes that selectively capture CO_2 have been shown to have high selectivity for CO_2 from a mixed gas waste stream and function well on nanoporous silica, however eliminating the silica layer could improve commercial manufacturability. We have proposed the use of enzyme treated nanoporous alumina alone, as an alternative to the enzyme treated silica/alumina layered material. This study sought to determine if alumina can function as well as silica as an enzyme treated surface for CO_2 capture. Quartz crystal microbalance (QCM) analysis was conducted to determine the amount of enzyme absorbed on the different alumina and silica substrates and UV-vis spectrophotometry was used in conjunction with colorimetric assays to determine the activity level of the enzymes on silica versus alumina. Understanding the interactions of the nanopore surface chemistry and enzyme stability is important in improving manufacturing processes leading to decreased costs, and improvements in chemical synthesis and waste treatment.

(P-T4)

Effect of Lewis Base on Electrochemical Behavior of Al Containing Ionic Liquid for Energy Storage

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The effect of an added Lewis base to an aluminum containing air-stable hydrophobic ionic liquid is examined as an attractive method for creating secondary Al-air batteries. Earth abundant aluminum based batteries are desirable for grid scale energy storage because of their theoretical high energy density and could be a safer and less expensive alternative to lithium batteries. However, the aluminum electrochemistry is not typically reversible and prevents the implementation of secondary Al-air batteries. Lewis base molecular additives were studied as possible candidates to help stabilize the aluminum electrochemistry. The electrochemical behavior of melts containing the Lewis base and melts without the Lewis base were experimentally found to dramatically differ in the observed electrochemical reversibility and reproducibility. The ionic liquid melts containing the Lewis base additive showed effective oxidation and reduction of the redox active aluminum molecular species allowing for effective cycling and preliminary results promise this to be a good candidate for future secondary Al-air batteries.

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(P-T5)

A Demonstration of Electron Microscopy at New Mexico Tech

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Electron microscopy is a powerful and flexible tool for characterization of natural and synthetic materials necessary in materials engineering and other disciplines. These instruments are adept at characterizing morphological surfaces and microstructures, identifying distinct phases to evaluate relationships, determining chemical compositions and visualizing how they change spatially, as well as determining the orientation and boundaries of crystalline grains.

The JEOL IT700HR field emission scanning electron microscope (SEM) located at New Mexico Tech is a modern, high resolution microscope capable of resolving particles on nanometer scales. The microscope is equipped with four detectors: secondary electron (SE), backscattered electron (BSE), energy dispersive spectroscopy (EDS), and electron backscatter diffraction (EBSD) detectors, allowing it to perform a large suite of analyses.

This SEM has been utilized at New Mexico Tech for the past two years, characterizing materials from numerous disciplines (metals, ceramics, earth sciences, chemical engineering, mechanical engineering, biology). We want to showcase data from our SEM to highlight its capabilities in order to better support researchers from regional universities and industry.

(P-T6)

Tradeoffs and Variability of Mechanical Properties in Cold Worked 21-9-6 Stainless Steel Bars

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Sub-standard yield stress in a batch of 21-9-6 stainless steel (Nitronic 40) bars was observed while other batches passed requirements. This material requires enhanced property uniformity due to its application in critical components and therefore has tighter restrictions on alloying elements. Using tensile testing, this study investigates the distribution of yield and ductility across bar geometry for three lots of material and is corroborated alongside Vickers microhardness profiles. Results show that yield strength increases with distance from the center of the bar, indicating that mid-radius properties do not conservatively represent the center. Therefore, select bars were cold worked using radial forging to 10% and 14% reductions in area for comparison. Some bars were cold worked in an attempt to increase yield strength at the center. Cold worked bars demonstrated increased microhardness, with the most significant changes occurring at the center. While hardness measurements effectively illustrate the spatial distribution of tensile properties, they are insufficient for screening yield requirements in conforming versus non-conforming materials. These findings highlight the tradeoffs between yield strength and ductility due to cold working, as well as the increasing variability in hardness along the outer diameter.

(P-P1)

Modeling Si/SiGe quantum dot variability induced by interface disorder

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Nano-scale quantum dot (QD) qubits in SiGe exhibit competitive quantum characteristics, e.g. long coherence times, required of future quantum information technologies. A challenge in developing the SiGe platform lies in understanding relationships between interface structure and quantum electronic properties. For example, atomic disorder at Si/SiGe interfaces is theoretically predicted to strongly modulate the conduction band valley spitting (VS). This atomic-scale interface structure-to-electronic-function relationship may be a determining factor in manufacturability of SiGe qubits. However, to simply measure, deconvolve, and visualize solid-embedded few-atomic-layer interface structures spanning any appreciable volume is extremely challenging. Interfacial atomic disorder descriptions that span over application-relevant ensembles are only partially tractable with post-synthesis microscopy (transmission electron microscopy) or tomography (atom-probe tomography), owing to issues such as image convolution and limited sampling volumes. To yield more comprehensive multiscale yet atomistic heterointerface descriptions, we use a multimodal microscopy approach. By convolving data from scanning tunneling microscopy and high-angle annular dark field scanning transmission electron microscopy, we reconstruct 3D interfacial atomic structure and employ an atomistic multi-valley effective mass theory to quantify qubit spectral variability. The results indicate (1) appreciable VS variability of ~50% owing to alloy disorder and (2) roughness-induced double-dot detuning bias energy variability of order 1–10 meV depending on well thickness. For measured intermixing, atomic steps have negligible influence on VS, and uncorrelated roughness causes spatially fluctuating energy biases in double-dot detunings, potentially incorrectly attributed to charge disorder. Our approach yields atomic structure spanning orders of magnitude larger areas than post-growth microscopy or tomography alone, enabling more holistic predictions of disorder-induced qubit variability and of significance for understanding performance limits in quantum electronics applications.

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(P-P2)

Exploration of the Structural-Property Relationship of Mn-Doped BF-BT for Ferroelectric Transducers

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Bismuth-ferrite barium-titanate (BF-BT) has experienced recent interest as a viable Pb-free alternative to lead zirconate titanate (PZT) explosive-electric transducers. Current devices exploit the pressure-induced phase transformation in PZT 95/5 from rhombohedral (ferroelectric) to orthorhombic (antiferroelectric) to produce current, with the same mechanism recently demonstrated in BF-BT. Over-reliance on Pb poses a challenge due to environmental health and safety regulations and limits agility in upgrading explosive-electric transducers. Here, we investigate the structure, processing, and electrical properties of compositions in the BF-BT solid solution for transducer applications. Implementation of BF-BT in this application have the potential to enable device use over a wider range of temperatures due to higher Curie temperature (Tc) (~450 °C) and reduced component weight and volume due to higher power density. However, preparation of BF-BT is challenging due to thermal instability of Bi and Fe as well as ancient understanding of structural-processing-properties for this system. To mitigate Fe reduction, we explore introduction of manganese (Mn) into BF-BT, to help stabilize the Fe^{3+} and increase resistivity. This research will discuss the structural-property relationship of BF-BT with Mn doping using X-ray diffraction, microscopy, and electrical characterization.

(P-P3)

Investigation of subthreshold leakage current & single-event effects in gate-all-around field-effect transistors

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Historically, field-effect transistors have proven to be resilient to radiation-induced displacement damage in the device channel. However, as device dimensions approach the order of tens of atoms, displacement effects are expected to become more pronounced due to significant alteration of the band structure and local density of states. We explore single-event displacement damage effects on subthreshold leakage current, drive current, and threshold voltage in gate-all-around field-effect transistors (GAAFETs), the leading candidate for next-generation CMOS devices. We perform focused ion beam (FIB) implantation of lithium ions into GAAFET devices, studying the gate drain current vs. gate voltage (ID-VG) relationship pre- and post-implantation to determine the minimum fluence required to have an observable effect on the subthreshold leakage current. We then systematically irradiate the devices with varying fluence, from below the minimal fluence required to have an observed effect to a maximum fluence which renders the device completely inoperative. We present measurements of the transport curves as a function of temperature, as well as noise spectroscopy measurements of irradiated and unirradiated devices as a function of the gate voltage. These measurements allow us to characterize the effect of displacement damage on device characteristics, defect types, and the defect energy levels by effectively altering the channel and device Fermi level with either gate voltage or temperature.

(P-P4)

Substrate dependence of heat dissipation in GaN p-n diodes bonded to SiC, AlN DBC, and diamond

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Vertical GaN power electronic devices are well-suited to power electronic applications due to their large band gap, electron saturation velocity, and thermal stability [1]. The applicability of GaN devices for national security missions and to power electronic applications more broadly is limited by GaN's thermal conductivity. Relative to AlN (2.85 W/cm·K), SiC (~3 W/cm·K), and diamond (22 W/cm·K), GaN (1.6 W/cm·K) dissipates heat inefficiently, leading to device failure at high power density. Further advancement of vertical GaN power devices requires engineered enhancement of heat dissipation. Metal compression bonding of thinned GaN films to more thermally conductive substrates is a promising potential solution to this challenge [2], taking advantage of the electrical characteristics of GaN with the superior thermal characteristics of a bulk foreign substrate, while allowing for a backside contact to the vertical device at the bonded interface.

Mapping the rates of heating and heat dissipation of GaN power devices bonded to thermally conductive foreign substrates is critical to assessing the degree to which thermal management can be improved. This work interrogates the heating and thermal conduction behavior in GaN p-n diodes bonded to bulk SiC, AlN direct bonded copper (DBC), and diamond substrates. Transient thermoreflectance measurements yield space- and time-resolved thermal conduction behavior in diodes in response to both pulsed and steady state biasing conditions. Using this method, heating behavior at sub-μm resolution at μs timescales is observed, and the variation of this behavior as a function of device power, bonded substrate, and bond quality is interrogated. Thermoreflectance results are directly compared to high-resolution infrared imaging. Minor discrepancies are observed between the methods, which will be discussed in conjunction with their complimentary nature for thermal characterization of devices. Device heat dissipation at a given power density is found to be proportional to the thermal conductivity of the substrate in well bonded regions

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[2] Felbinger, Jonathan G., et al. "Comparison of GaN HEMTs on diamond and SiC substrates." IEEE Electron Device Letters 28.11 (2007): 948-950.

(P-P5)

Microstructure/Performance Investigation of HDPE composite in Thermal and Irradiation Environments

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Commercial high-density polyethylene (HDPE) is hydro carbonic in nature having linear structure, light weight, excellent mechanical properties, and good chemical resistance. HDPE have limited uses for extreme environment due to hydro carbonic nature and low thermal stability. One method to enhance the thermal stability is to mix other materials with high thermal stability. Lanthanide-based nanomaterials (Ln_2O_3) possess unique properties such as high melting point and various electromagnetic interactions. Typically, sedimentation and agglomeration plague HDPE nanocomposites. Therefore, to alleviate this issue, the twin screw extruder was utilized to achieve good dispersion and decent loading levels. This paper presents the fabrication of HDPE composite with various loading of Ln_2O_3 as well as the microstructure characterization as a function of processing variable (i.e., loading, heating). Thermal functionality was evaluated as a function of loading as well as preliminary gamma radiation dose effect on physical and chemical properties HDPE nanocomposites.

(P-P6)

Tungsten-based alloys for fusion reactor materials

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Many efforts have been made to design the next fusion reactor materials that can withstand extreme radiation and temperature, while performing at a high level. Tungsten (W) is currently the leading candidate material used in various fusion energy reactor components due to high melting point, high sputtering resistance and thermal shock resistance. However, it has poor oxidation resistance and radiation induced embrittlement causing voids leading to degradation of material properties.

Mechanical alloying of W with other transition metals is one method to enhance oxidation and radiation properties by introducing grain boundaries that act as defect sinks that can serve as sources to emit interstitials and annihilate vacancies, that potentially reduce the radiation induced embrittlement, as well as other property enhancement.

In this work, we discuss the synthesis/processing of Tungsten alloys via vacuum arc melting of various W:TM composites (TM= Ta, Nb, Ti) at different composition to understand the microstructural evolution. The correlation of the microstructure (SEM- EDS), mechanical properties, structural phase (XRD), and densification.

(P-P7)

Self-diffusion of Volatile Organic Compounds in Zr-MOFs

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The association of specific volatile organic compounds (VOCs) in exhaled human breath (EHB), often called a chemical “fingerprint”, to a particular disease is a growing field of study. The ability of trained scent dogs to identify COVID-positive respiratory secretion samples lends itself to the possibility of developing a non-invasive, breath-based diagnostic tool to provide insight into a person’s state of health. However, detecting the target constituents --- often existing at dilute concentrations in a complex mixture of water, CO_2, and other VOC interferents --- poses a significant challenge.

Metal-organic frameworks (MOFs) have demonstrated tremendous aptitude for applications in gas sensing and separation technologies. MOFs are porous, crystalline solids composed of metal nodes coordinated by organic linkers which form an extended network. Zirconium (Zr) MOFs exhibit exceptional thermal and hydrolytic stability which makes them attractive candidates for studying VOC detection in EHB. If MOFs are to be used in a beath-based diagnostic tool, understanding the interactions between the VOCs and the MOF is vital.

In this work, we use molecular dynamics simulations and experimental NMR to study the self-diffusion properties of several polar and non-polar VOCs in a topologically diverse set of Zr-MOFs. We compute self-diffusion coefficients at multiple loadings over a range of temperatures and compare against experimental values. We will discuss trends between self-diffusion and heat of adsorption, molecular properties (e.g. chain length, polar or non-polar, and isomers), and framework topology. Finally, we consider the challenges of comparing simulation to NMR experiments.