The 31st Rio Grande Symposium on Advanced Materials

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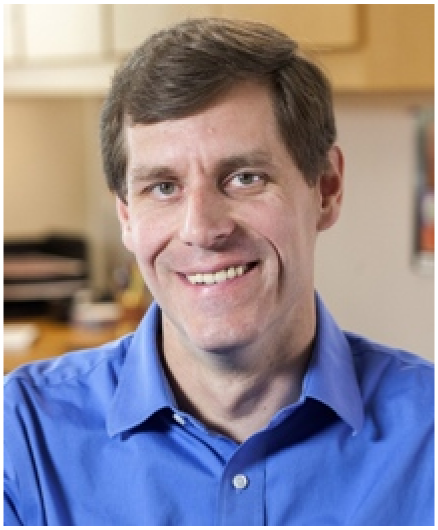
	Potters	**Turquoise**	**Weavers**
8:00am	Registration & Exhibition (Franciscan)		
9:00am	Catalysis & Surfaces: Davis-Wheeler Chin Choudhuri Noureddine Henkelis Datye	2D Materials: Spoerke Ruiz Yoo Tung	Soft Additive Materials: Roberson O'Connor Secor Scheideler
10:45am	Break		
11:00am	Kreidl Lecture, Professor Mark Hersam (Franciscan, lunch provided)		
1:00pm	Student Competition: Arnot Kunwar Canning Pan Reuel Tang DiGregorio	Mechanical Properties: Khraishi Choudhuri Laursen Chabi Deibler White	Energy Storage: Baca Spoerke Rodriguez Lim
2:30pm	Break		
2:45pm	Semiconductor Devices: (Begins at 3:00) Titze Yates Manuel	Solution Chemistry: Fowler Vogel Johnston Bell	Ceramic & Structural Materials: Bell Strong Clark
3:45pm	Poster Session (Fire Place Room)		
5:00pm	Awards Presentation & Closing		

Kreidl Memorial Lecture

Norbert J. Kreidl

The Kreidl Memorial Lecture honors the career achievements of Norbert Kreidl, a remarkable and indefatigable glass scientist who spent his final years as a consultant based in Santa Fe, New Mexico.



Mark C. Hersam

Walter P. Murphy Professor of Materials Science and Engineering, Department of Materials Science and Engineering, Northwestern University

Mark C. Hersam is the Walter P. Murphy Professor of Materials Science and Engineering and Director of the Materials Research Center at Northwestern University. He also holds faculty appointments in the Departments of Chemistry, Applied Physics, Medicine, and Electrical Engineering. He earned a B.S. in Electrical Engineering from the University of Illinois at Urbana-Champaign (UIUC) in 1996, M.Phil. in Physics from the University of Cambridge (UK) in 1997, and a Ph.D. in Electrical Engineering from UIUC in 2000. His research interests include nanomaterials, nanomanufacturing, scanning probe microscopy, nanoelectronic devices, and renewable energy. Dr. Hersam has received several honors including the Presidential Early Career Award for Scientists and Engineers, TMS Robert Lansing Hardy Award, AVS Peter Mark Award, MRS Outstanding Young Investigator, U.S. Science Envoy, MacArthur Fellowship, and eight Teacher of the Year Awards. An elected member of the National Academy of Inventors, Dr. Hersam has founded two companies, NanoIntegris and Volexion, which are commercial suppliers of nanoelectronic and battery materials, respectively. Dr. Hersam is a Fellow of MRS, AVS, APS, AAAS, SPIE, and IEEE, and also serves as an Associate Editor of ACS Nano.

Kreidl Lecture Abstract

Mixed-Dimensional van der Waals Heterostructures for Electronic and Energy Applications

Layered two-dimensional (2D) materials interact primarily via van der Waals bonding, which has created new opportunities for heterostructures that are not constrained by epitaxial growth [1]. However, it is important to acknowledge that van der Waals interactions are not limited to interplanar interactions in 2D materials. In principle, any passivated, dangling bond-free surface interacts with another via non-covalent forces. Consequently, layered 2D materials can be integrated with a diverse range of other materials, including those of different dimensionality, to form mixed-dimensional van der Waals heterostructures [2]. Furthermore, chemical functionalization provides additional opportunities for tailoring the properties of 2D materials [3] and the degree of coupling across heterointerfaces [4]. In order to efficiently explore the vast phase space for mixed-dimensional heterostructures, our laboratory employs solution-based additive assembly [5]. In particular, constituent nanomaterials (e.g., carbon nanotubes, graphene, transition metal dichalcogenides, black phosphorus, boron nitride, and indium selenide) are isolated in solution, and then deposited into thin films with scalable additive manufacturing methods (e.g., inkjet, gravure, and screen printing) [6]. By achieving high levels of nanomaterial monodispersity and printing fidelity [7], a variety of electronic and energy applications can be enhanced including digital logic circuits [8], photodetectors [9], and lithium-ion batteries [10,11]. Furthermore, by integrating multiple nanomaterial inks into heterostructures, unprecedented device function is realized including anti-ambipolar transistors [12], gate-tunable photovoltaics [13], and neuromorphic memtransistors [14]. In addition to technological implications for electronic and energy technologies, this talk will explore several fundamental issues including band alignment, doping, trap states, and charge/energy transfer across previously unexplored mixed-dimensional heterointerfaces [15].

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[2] D. Jariwala, et al., Nature Materials, 16, 170 (2017).
[3] C. R. Ryder, et al., Nature Chemistry, 8, 597 (2016).
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[7] J. Kang, et al., Accounts of Chemical Research, 50, 943 (2017).
[8] M. Geier, et al., Nature Nanotechnology, 10, 944 (2015).
[9] J. Kang, et al., Advanced Materials, 30, 1802990 (2018).
[10] K.-S. Chen, et al., Nano Letters, 17, 2539 (2017).
[11] W. J. Hyun, et al., ACS Nano, DOI: 10.1021/acsnano.9b04989 (2019).
[12] V. K. Sangwan, et al., Nano Letters, 18, 1421 (2018).
[13] D. Jariwala, et al., Nano Letters, 16, 497 (2016).
[14] V. K. Sangwan, et al., Nature, 554, 500 (2018).
[15] S. B. Homan, et al., Nano Letters, 17, 164 (2017).

ORAL PRESENTATIONS

ORAL

Functionalized Poly(phenylene) for Advanced Electrochemical Process Applications

Ehren Baca[1], Cy Fujimoto[1], Michael Hibbs[1], Sandip Maurya[2], Albert S. Lee[2], Dongguo Li[2], Eun Joo Park[2], Yu Seung Kim[2]

1. Sandia National Laboratory
2. Los Alamos National Laboratory

Electrochemical processes have the promise to offer efficient and scalable solutions to challenges faced in energy production, energy storage, water treatment and advanced manufacture. Such processes are either dependent on, or enhanced by, the implementation of ion conducting materials acting as in-situ ion transport facilitators or inhibitors. Desirable properties of ion exchange materials are amenability to both cation and anion functionalization, high and low pH stability, physical and mechanical durability, high ion conductivity and tailorable ion exchange capacity. Sandia's Diels-Alder poly(phenelyne) developed by Fujimoto et al. [1] possess these qualities as a scalable, cost effective hydrocarbon polymer backbone. Furthermore, Hibbs [2] showed that Fujimoto's material can be acylated with a hexamethylene spacer to accept a quaternary ammonium cation achieving one of the most robust anion exchange membranes currently available. A testament for the diverse range of applications of functionalized poly(phenylene) is evidenced by the promising results achieved by this material in both anion exchange membrane fuel cells (AEMFC) and high temperature proton exchange membrane fuel cells (HT-PEMFC). It has been shown by Kim et al. [3] that phosphoric acid doped quaternary ammonium tethered poly(phenylene) outperforms Nafion in HT-PEMFC due to a wider operating window of both temperature and relative humidity. Efforts to further develop Fujimoto's material for applications in other sectors such as flow batteries, electrolyzers, the hybrid sulfur cycle and water treatment are currently underway at Sandia National Laboratory and will be discussed in this talk.

[1] Fujimoto, C. H., Hickner, M. A., Cornelius, C. J., & Loy, D. A. (2005). Ionomeric poly (phenylene) prepared by Diels− Alder polymerization: synthesis and physical properties of a novel polyelectrolyte. Macromolecules, 38(12), 5010-5016.

[2] Hibbs, M. R. (2013). Alkaline stability of poly (phenylene)-based anion exchange membranes with various cations. Journal of Polymer Science Part B: Polymer Physics, 51(24), 1736-1742

[3] Lee, K. S., Spendelow, J. S., Choe, Y. K., Fujimoto, C., & Kim, Y. S. (2016). An operationally flexible fuel cell based on quaternary ammonium-biphosphate ion pairs. Nature energy, 1(9), 16120.

ORAL

Polymer Intercalation Synthesis of GlycoBoehmite Nanosheets

Nelson Bell, Mark A. Rodriguez, Jessica N. Kruichak, Bernadette A. Hernandez-Sanchez, Manuel Casillas, Igor Kolesnichenko, Paul Kotula, Edward Matteo
Sandia National Laboratories

Novel alumina nanosheets based onthe aluminum oxyhydroxide boehmite phases were prepared using glycothermal routes, in which the boehmite phase is altered by chemisorption of the glycol solvent in place of the interlayer hydroxyl groups, creating glycoboehmite. Two new phases that incorporate either polyvinylpyrrolidone or hydroxylpropyl cellulose polymers were found to expand the b-axis of the unit cell beyond the value created from synthesis in the glycothermal solvent itself. These intercalation polymers are non-ionic and interact by wetting interactions and hydrogen bonding, rather than by chemisorption or chelation with the aluminum ions in the structure. The ion absorption capacity was evaluated for environmental remediation applications of these materials.

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ORAL

Controlling Shear Thickening in SiC Suspensions using Surface Chemical Modification

Nelson Bell, Joshua R. Boykin, Bernadette A. Hernandez-Sanchez
Sandia National Laboratories

Shear thickening fluids (STFs) are non-Newtonian fluids which undergo an increase in viscosity with increasing shear rate, and are useful for shock mitigation and physical protection. Recent theoretical and modeling reports have identified the influence of hydrogen bonding from surface chemistry as the critical factor in developing high shear thickening performance. This has lead to the dominance of SiO2 particles in STFs over less hydrophilic particles such as SiC, which are harder and have greater acoustic impedance. This work tests the hypothesis that surface modification using polymer surfactants can control the formation and extent of shear thickening properties for SiC, to achieve tailorable viscosity performance in advanced STF systems. Poly(vinyl alcohol) (PVA), poly(vinyl pyrrolidone) (PVP), poly(ethylene imine) (PEI), polydopamine (PD), and cellulose acetate (CA) were used as dispersants. PVP, PEI, PD, and CA were found to be effective dispersants, allowing for higher volume fractions to be reached. PD@SiC and CA@SiC were successfully used in conjunction with poly(ethylene glycol) MW=400 (PEG400) to produce STFs with appreciable shear thickening behavior.

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ORAL

Understanding Structure-Mechanical Properties Relations in Kevlar® Single Fiber

Sakineh Chabi[1], Fei Ren[2]
1 Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM, 87131
2 Department of Mechanical Engineering, Temple University, Philadelphia, PA, 19122

This study aims to elucidate the relationship between the mechanical properties and microstructures of Kevlar® fibers at the micro/nano scale. The skin-core structure of Kevlar® 29 fiber was revealed through a focused electron beam experiment inside a scanning electron microscope (SEM) chamber. Cross sectional SEM images of the broken fiber showed that the thickness of the skin ranged from 300 to 800 nm and that the core region consisted of highly packed layers of fibrils. The skin and the core regions showed different mechanical behaviour and structural changes during nanoindentation and micro-tensile tests, indicating that the core region possessed higher stiffness, whereas the skin region could undergo more plastic deformation. Furthermore, micro-tensile testing results showed that the ultimate tensile strength, the elongation at failure, and the tensile toughness of single fibers could be significantly enhanced by cyclic loading. Such findings are important to understand the contribution of different microstructures of Kevlar® fibers to their mechanical performance, which in turn can be utilized to design high-performance fibers that are not limited by the trade-off between toughness and stiffness.

ORAL

Deformation of interface dominated multiphase materials

Deep Choudhuri
New Mexico Institute of Mining and Technology

Multicomponent high *entropy* alloys were originally designed to form a single-phase solid solution. However, several recent studies have shown that *positive enthalpy effects,* i.e. attraction between dissimilar atoms, lead to the formation of various intermetallic compound (IMC) phases. Here, we will present results from a promising IMC-reinforced HEA microstructure that comprises of fcc-matrix and bcc-ordered B2 IMC. The structure of fcc/B2 semicoherent Kurdjumov-Sachs (KS) interface was rigorously determined by coupling molecular dynamics (MD) simulations, TEM and electron-backscattered diffraction (EBSD). Furthermore, MD simulations, involving the deformation of near-realistic fcc-B2 microstructures, were conducted to reveal the role of KS interface on deformation mechanisms. These simulations established a direct relationship between the structural features in the KS interface and deformation processes like twin formation within fcc phase, fcc-to-B2 slip transfer and fcc/B2 interfacial strain accumulation.

ORAL

Influence of local lattice-level covalent character on diffusion and phase formation in a highly creep-resistant Mg-Nd-Zn alloy

Deep Choudhuri
New Mexico Institute of Mining and Technology

Creep behavior is a key design consideration for deploying Mg alloy in automotive applications. Here we report a substantial – an order of magnitude – improvement in creep strength by adding only a minor quantity of Zn to a Mg-Nd alloy. High resolution microscopy indicated that the resulting microstructure contained high volume fraction of fine-scale precipitates on the {0001}-basal planes of Mg, and also on the {01-10}/{11-20} prismatic planes. To obtain a deeper understanding of such a creep-resistant microstructure; the electronic structures of precipitates, precipitate/matrix interfaces and solid solutions were examined via density functional theory (DFT) based first principles calculations. Our DFT results indicated that anisotropic distribution of electron charge densities, or the bonding character play a vital role in determining the creep-strength of Mg alloys. From the standpoint of our experimental observations, we will discuss the role of differing bonding characters on vacancy diffusion and precipitate phase formation on creep-deformation

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ORAL

Evolution of He nanobubbles and nanocavities in Palladium

Trevor Clark[1], Caitlin Taylor[1], David Robinson[2], Joshua Sugar[2], Khalid Hattar[1]
1 Sandia National Laboratories, Albuquerque NM
2 Sandia National Laboratories, Livermore CA

Materials exposed to the extreme radiation and temperature inside current and future nuclear reactors accumulate helium generated by nuclear reactions, which tends to form nanobubbles that grow and coalesce; this can result in embrittlement and mechanical failure of the material. In this work in situ ion irradiation transmission and scanning electron microscopy experiments are used to emulate these extreme conditions to enable real time observation of microstructural evolution at the nanoscale. Nanocrystalline palladium is selected as a high purity model FCC system to investigate the complex interactions and evolution of grain boundaries, nanobubbles, and nanocavities as a function of both irradiation conditions and temperature. This presentation will discuss cavity growth mechanisms for various homologous temperature regimes and the complex interaction of cavities with grain boundaries. The results of this and future work will lead to insight into the underlying mechanisms and physics governing this evolution and inform predictive models necessary for reliable materials design.

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ORAL (INVITED)

Atom Trapping: Key to the Design of Thermally Stable and Regenerable Single Atom Catalysts

Abhaya Datye
Department of Chemical and Biological Engineering, University of New Mexico

Heterogeneous catalysts represent the mainstay of the chemical industry, and a large majority involve nanoparticles on a support. Decreasing size of the nanoparticles leads to better utilization of the precious metals, with the highest atom efficiency being achieved when the metal is atomically dispersed in the form of isolated atoms. Isolated atoms become mobile at elevated temperatures, causing agglomeration into nanoparticles. Our research is focused on developing methods to control the growth of particle size and the transformation of nanoparticles into isolated single atoms. Supports differ in their ability to maintain small particles. For instance, if we prepare 1 wt% Pt synthesized using the same amine precursor and calcined at 500 °C in air to decompose the precursor, the resulting catalysts are very different. The conventional term used to describe these differences is metal-support interactions (MSI), which is meant to suggest bonding of the metal nanoparticle with the oxide support. But the term MSI fails to capture the underlying mechanism that leads to these observations. We have characterized these differences in catalyst supports in terms of their ability to trap atoms. We learnt that ceria supports help generate a stable and fully regenerable Pt catalyst that can change reversibly from single atoms into metallic nanoparticles. The understanding of atom trapping derived from ceria supports can be translated to other oxide supports. This will impact not only automotive exhaust treatment (where catalysts are exposed to high temperature) but also other industrial reactions such as propane dehydrogenation or methane oxidation, where high temperatures are required.

ORAL

Facile Microwave Synthesis and Surface Modification of Rare Earth Oxide Nanospheres for Dispersion in Polymer Matrices

Clare Davis-Wheeler Chin and LaRico J. Treadwell
Sandia National Laboratories

A facile new microwave route for the synthesis of small (~ 5 nm), dispersible rare earth oxide nanoparticles (RE_2O_3 NPs; RE = Ce, Er, Gd, Nd, Pr, Sm) has been developed. Rare earth precursor nanospheres with monodispersed size and morphology were produced in high yield via 10 minute microwave (MW) reaction that utilizes low cost, environmentally friendly reagents. Topotactic conversion from the precursor material to the rare earth oxide (RE_2O_3) is performed by heating the as-synthesized precursor material in air. Characterization of both the precursor and RE NPs composition and morphology was conducted via powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), and transmission electron microscopy (TEM). Results indicate that while heating the precursor induces compositional conversion, the morphology and size of the NPs is unaffected.

Silane surface modification of the RE_2O_3 NPs for optimizing polymer entry was also conducted via facile MW route. RE_2O_3 NPs were functionalized with one of four different silanes in order to examine the effect of silane chain length and substitution on the dispersibility of the modified NPs within different polymer matrices. Surface treatment of the RE_2O_3 NPs with 3-aminopropyltrimethoxysilane (APTMS), triethoxymethylsilane (MTM), triethoxy(octyl)silane (OTEOS), or tetraethoxysilane (TEOS) was performed by refluxing suspensions of RE_2O_3 NPs and each silane under MW irradiation. Confirmation of silane surface modification was carried out via Fourier transform infrared spectroscopy (FTIR) and TGA.

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ORAL

Influence of microstructure, stress, and temperature on the behavior of springs over time

Lisa Deibler, John Laing, Christopher Finfrock, Aron Robbins
Sandia National Laboratories, Albuquerque, NM, USA

Stress relaxation in springs is a phenomenon that is temperature, time, stress, and microstructure dependent. In this work I examine how two different alloy springs, one compression spring and one tension spring, respond to various temperatures and stress levels for aging periods of 1-2 years. We also examine how the differences in microstructure between the two alloys and springs may influence their time-dependent response. Finally, I compare the measured stress relaxation with the requirements for the parts over 30 years and determine whether the springs will likely meet requirements under normal operating conditions.

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ORAL

Surface chemistry of the frog sticky-tongue mechanism

James Elliott Fowler [1,2], Thomas Kleinteich [3], Johannes Franz [4], Cherno Jaye [5], Daniel A. Fischer [5], Stanislav N. Gorb [3], Tobias Weidner [4,6], Joe E. Baio [2]
1. Sandia National Laboratories, Albuquerque, NM 2. Oregon State University, Corvallis, OR
3. Zoological Institute of the University of Kiel, Kiel, Germany 4. Max Planck Institute for Polymer Research, Mainz, Germany 5. National Institute of Standards and Technology, Gaithersburg, Maryland
6. Aarhaus University, Aarhaus, Denmark

Frogs capture their prey with a highly specialized tongue. Recent studies indicate this tongue is covered with fibril-forming mucus that acts as a pressure sensitive adhesive. However, no analysis of the interfacial chemistry of frog tongue mucus has been performed. The goal of this study is to examine the chemical structure of the surface of mucus after a tongue strike. Previous studies of mucus from other animals suggest that mucus from a frog's tongue consists of mucins—serine-, threonine-, and proline-rich glycoproteins. Therefore, the authors expect to observe chemical bonds associated with glycoproteins, as well as fibrils formed at the mucus–tongue interface.To test this hypothesis, they collected both near-edge x-ray absorption fine structure (NEXAFS) microscopy images and sum frequency generation (SFG) vibrational spectra from layers of mucus left after frog tongue strikes on cleaned glass slides. NEXAFS imaging demonstrates a uniform distribution of amide, hydroxyl, and carbon–carbon bonds across the mucus surface. Difference spectra of individual N1s and C1s K-edge spectra pulled from these images indicate a structure consistent with fibril formation as well as disorder of oligosaccharide groups near the mucus surface. C—H region SFG spectra reveal surface active modes which likely stem from serine and threonine within the mucin protein. Combined, this work suggests that glycoproteins are well-ordered at the mucus–tongue interface. Published by the AVS.

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ORAL

Acid Gas Stability and Selectivity of Rare Earth MOFs

Susan E. Henkelis, Tina M. Nenoff, Dorina Sava Gallis, Grace Vincent, D. Jon Vogel
Sandia National Laboratories, Albuquerque, NM 87185, USA

Herein, we report on the novel application and study of isostructural metal-organic framework (MOF) materials platform based on RE-DOBDC (RE= Y, Yb, Tb, Eu; DOBDC= 2,5-dihydroxyterephthalic acid) containing coordinatively unsaturated open metal sites (CUSs). In particular, we are interested in understanding the structural and thermal stability of these analogs to caustic gases (NO_x, SO_x). To do this, we investigated the preferential adsorption of these gases as function of metal identity and examined their performance in complex gas environments. The MOFs were synthesized under solvothermal conditions and fully characterized by XRD, BET, FTIR and photoluminescence. Bulk gas studies involved NO_x generation in an adsorption chamber at room temperature. Each MOF was shown to retain their structural integrity under NO_x exposure. Interestingly, pre-NOx exposure these MOFs exhibit photoluminescence under UV light. However, upon NOx exposure, that emission is quenched. This is indicative of stimuli responsive nature in this multifunctional material.

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ORAL

Anti-CRISPR Based Platform for Rapid Detection and Quantification of Cas9-RNP

Robert Johnston
Nanobiology Department, Sandia National Laboratories, Albuquerque, NM, USA

The demonstration of RNA-guided DNA editing using the clustered regularly interspaced short palindromic repeats (CRISPR)/CRISPR-associated (Cas) system spawned a new era in biotechnology. The facile, programmable nature of gene editing afforded by CRISPR/Cas9 has led to a multitude of application in both the lab and the clinic. In these applications, detection of the CRISPR/Cas9 RNP within biological samples is critical for assessing gene-editing reagent delivery, retention, persistence, and distribution within living organisms to optimize editing while minimizing the potential for off target or other deleterious effects. Traditional biochemical-based detection methods (Western blot, ELISA), while effective, are either time consuming, expensive, or are only semi-quantitative, necessitating development of more rapid and precise analytical methods for detection of CRISPR components. Herein, we present development of a rapid bioassay platform for quantitative Cas9-RNP detection using the anti-CRISPR protein, AcrIIA4 as a novel affinity reagent. Glassy carbon electrode surfaces were functionalized via electrodeposition of aryl nitrodiazonium salts. Post functionalization, cysteine modified AcrIIA4 was attached to electrode surfaces via a heterobifunctional crosslinker. Using this platform, we demonstrate detection CRISPR/Cas9 RNP by, fluorescent, colorimetric, and electrochemical methods in less than 3 hours, achieving detection limits of 280 pM RNP in reaction buffer and 8 nM RNP in biologically representative conditions via electrochemical measurements. Our results demonstrate the ability of anti-CRISPR proteins to serve as robust, specific, flexible, and economical CRISPR/Cas9 recognition elements for developing precise, rapid, and economical biosensing devices for CRISPR/Cas9 RNP detection.

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ORAL

A More Generalized Method for the Interaction of Dislocations with Free Surfaces

Tariq Khraishi, Abu Bakar Siddique
Mechanical Engineering Department, University of New Mexico

A common problem in dislocation dynamics simulations is the proper treatment of boundary conditions. Here, the authors present a more generalized method to treat traction-free surfaces nearby dislocations. This is a collocation point method where these points are the centers of dislocation loops distributed on the free surface. The Burgers vectors for such loops is solved for and this enables the enforcement of zero traction at the collocation points. Verification of this method as well as ensuing simulations are presented.

ORAL

The Effect of Various Geometrical Flaws on Additive Manufactured Component Performance

Christopher Laursen[1], Jay Carroll[1], Jody Bartanus[2], Benjamin Smith[2], Garrett Pataky[2]
1 Sandia National Laboratories, Albuquerque, NM, USA
2 Clemson University, Department of Mechanical Engineering, Clemson, SC, USA

Developments in additively manufactured (AM) components continue to harbor a high number of flaws even with global enhancements in manufacturing methods; yet a certain number of flaws will be acceptable within component requirements. The overarching goal of this study is to develop a method for identifying different disqualifying flaw types and designating an acceptable threshold within these flaw types. The criticality of a flaw can vary throughout a part and will be dependent on inherent material properties the component is composed of. In this work two AM alloys with drastically different mechanical behavior, 316 stainless steel and AlSi10Mg, were chosen for testing in an exemplar component which included various, intentionally introduced geometric flaws. These properties were then compared to baseline experiments in tension, compression, fracture toughness, etc. performed on adjacent test coupons. The interaction between intentional flaws with inherent material properties, component geometry, and other flaws is examined. In the end, this work hopes to define a new paradigm for qualification of AM components with known flaws.

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ORAL

Effect of ZnO-Saturated Electrolyte on Rechargeable Alkaline Zinc Batteries at High Depth-of-Discharge

Matthew Lim, Igor Kolesnichenko, David Arnot, Timothy Lambert
Sandia National Laboratories, Albuquerque, NM, USA

Rechargeable alkaline MnO_2–Zn and Ni–Zn batteries are potential low-cost, safe energy storage technologies for grid applications. However, the Zn anodes suffer from redistribution and passivation of active material over repeated cycling, leading to capacity loss. One proposed solution is to pre-saturate the electrolyte with ZnO to minimize dissolution and long-range migration of zinc from the anode. While not a novel concept, most of the relevant literature uses flooded cells and disregards the large excess of Zn species in the electrolyte relative to the anode, which inflates the specific capacity.

Here, we investigate the effect of ZnO-saturated electrolyte in more commercially relevant, non-flooded Ni–Zn cells at high Zn depth-of-discharge (DOD_{Zn}). Cells at tested at 14%, 21%, and 35% DOD_{Zn} with ZnO-saturated KOH electrolyte exhibit 191%, 235%, and 110% longer cycle life respectively over identically tested cells with ZnO-free electrolyte, even when the DOD accounts for dissolved ZnO. We also study ZnO saturation with anodes containing $Ca(OH)_2$ and Bi_2O_3 additives, which have previously been shown to improve cycle life at 15% DOD_{Zn} in additive-free electrolyte.

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ORAL

Investigation of displacement damage induced leakage and annealing effects of SiC Schottky diodes

Jack Manuel, Barney Doyle, Gyorgy Vizkelethy, Bastiaan Vaandrager, Edward Bielejec
Sandia National Laboratories

Sandia National Laboratories (SNL) is interested in the operation of wide bandgap semiconductors, including SiC, GaN, and AlGaN, in hostile environments consisting of neutron induced displacement damage, total ionizing dose and dose rate effects. Ion and electron beam irradiation provides a method of simulating these hostile conditions and offers the benefits associated with the ability to focus, pulse, and regulate the flux of the charged particles. Our experiments show that ion beam induced degradation of Silicon Carbide (SiC) Schottky diodes causes increased reverse bias leakage current while leaving forward characteristics unchanged. This effect is explored using common characterization techniques such as I-V, C-V and DLTS measurements. Additionally, SNL is concerned with early time annealing. We present a novel method of investigating early time annealing effects combining probing electron beam pulses (EBIC) within the temporal vicinity of an ion induced displacement damage. We observe a clear late time annealing signature and we are investigating the origin of the early time annealing.

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ORAL

Ligand-Free Ultrasmall Metal Nanocluster Catalysts Confined in Mesoporous Silica Nanoparticles

Achraf Noureddine[1], Wei Zhu[1], Jane Howe[2], Jimin Guo[1], Jeffrey Brinker[1]
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Supported ultrasmall noble metal nanocluster-based (UNMN-based) catalysts are one of the most important classes of solid materials for heterogeneous catalysis. In this work, we present a novel strategy for the controlled synthesis of ligand-free UNMN nanocatalysts based on in situ reduction of a palladium based (Pd based) metal−organic cage (MOC) confined within monosized, thiol-modified mesoporous silica nanoparticle (MSN) supports. By taking advantage of the high mutual solubility of MOCs and MSNs in DMSO and the strong interactions between the thiol-modified MSN pore wall and MOC surface, a good dispersion of MOC molecules was achieved throughout the MSN support. The close correspondence of the MSN pore diameter (ca. 5.0 nm) with the diameter of the MOC (ca. 4.0 nm) confines MOC packing to approximately a monolayer. Based on this spatial constraint and electrostatic binding of the MOC to the thiol-modified MSN pore surface, in situ MOC reduction followed by metal atom diffusion, coalescence, and anchoring on the active sites resulted in ligand-free Pd-based UNMNs of approximately 0.9 ± 0.2 nm in diameter decorating the MSN pore surfaces. Control experiments of the reduction of a conventional palladium source or the reduction of free, unconstrained cages in solution under the same conditions only produced large metal nanocrystals (NP, >2 nm), confirming the importance of confined reduction to achieve a highly catalytically active surface. In light of this strategy, two catalytic experiments including the reaction of 4-nitrophenol to 4-aminophenol and the Suzuki C−C coupling reaction show superior catalytic activity of the engineered MSN-supported UNMN nanocatalysts compared to their free form and state of the art commercial catalysts. We believe that our new strategy will open new avenues for artificially designed UNMN-inspired nanoarchitectures for wide applications.

ORAL

Relating Molecular Architecture to the Extensional Rheology of Flowing Polymers

Thomas O'Connor
Sandia National Laboratories

Many industrial processes elongate polymer liquids at rates much faster than the molecule’s characteristic relaxation times. These nonlinear elongation flows can strongly deform microscopic polymer conformations and drive dynamic transitions that produce large changes in polymer viscosity. Understanding how flow depends upon and drives such changes in polymer microstructure is essential for improving established and emerging fabrication methods like fiber spinning and 3D printing. However, most microscopic understanding of these nonlinear flows has been drawn from indirect techniques that infer molecular dynamics from macroscopic rheology. This has begun to change with the recent development of new experimental and numerical simulation techniques that allow researchers to control, sustain, and microscopically probe polymer dynamics during strong elongational flows. Here, I’ll present molecular simulations for linear, branched, and ring polymer liquids deformed in uniaxial elongational flow. Molecular simulations reproduce rate dependent trends in viscosity that are measured in elongation experiments and reveal the microscopic dynamics driving them. I’ll show where simple theoretical arguments can directly relate the conformations of elongated molecules to their extensional viscosity and discuss extending these ideas to more complex polymers.

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ORAL (INVITED)

Tunable Polymeric Material Systems for the Advancement of Material Extruision 3D Printing

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2. Department of Metallurgical, Materials and Biomedical Engineering, UTEP

Though over twenty years old, the 3D printing technology of material extrusion additive manufacturing, also known as fused deposition modeling, relies mainly on off the shelf thermoplastic material systems that have been minutely tweaked to be compatible with the platform. The technology could be rapidly expanded through the adoption of novel material systems with a wider array of physical properties. Two strategies for creating novel material systems have been generally employed: 1) the development of novel polymer blends and; and 2) the development of novel polymer matrix composites. To reach the full potential, any developed material system should have a physical property that is tunable. The following work entails the development of three material systems with three distinct tunable properties: 1) radiation shielding; 2) toughness; and 3) shape memory. Motivation behind the development of each material system is presented. Materials characterization efforts including mechanical testing and electron microscopy are also highlighted. The end result is a demonstration of increasing the applicability of material extrusion additive manufacturing through the development of novel material systems.

ORAL (INVITED)

Detection of residual macrostrain in Li metal thin films via Tilt-A-Whirl methodology and a Be-dome specimen holder

Mark A. Rodriguez, Katharine L. Harrison, Brian Perdue, James J. M. Griego, Subrahmanyam Goriparti, Brad Boyce and Zach Casias
Sandia National Laboratories

The presence of residual strain plays an important role in materials properties and potential failure mechanisms. Currently we are investigating the role of strain in Li films for use in Li batteries; the magnitude of in-plane strain and compressive/tensile nature of the strain field may impact battery performance. As these films are highly reactive in air, we must maintain an inert environment around the sample during our X-ray analysis. Therefore, we have isolated the films within a special Be-dome specimen holder [see Rodriguez, et al. (2008) Powder Diffraction, 23, pp. 121-124] to prevent air exposure of the film while the diffraction measurement is performed. We have developed a protocol to characterize the presence of residual strain on various materials by employing an in-house Matlab-based texture analysis software package termed “TILT-A-WHIRL” [see Rodriguez, et al. (2013) Powder Diffraction, 28, pp. 81-89] which includes methods for macrostrain analysis via the $\sin^2$(⍰) technique. We present macrostrain results and the simultaneous texture analysis of Li filmsgenerated using different deposition conditions. We will present our results in the context of battery performance and detail the challenges of this unique sample preparation regarding alignment, while outlining the diffraction artifacts in the collected datasets and how they are dealt with when analyzing the data.

ORAL

High Energy Ion and Gamma Detection using the Graphene-Insulator-Semiconductor Junction

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Graphene’s atomically thin nature, high mobility and low intrinsic carrier concentration make it an ideal charge sensing material, particularly in the deeply depleted graphene-insulator-semiconductor (D^2GOS) junction architecture. Previously the D^2GOS has proven to be a highly sensitive to visible and near infrared light, resulting in high responsivity and high signal to noise rations; However, the D^2GOS is agnostic to the type of ionizing radiation. Here in this work we test the D^2GOS junction’s sensitivity to high energy Si^+ ions and gamma radiation, through real time detection of the ionizing radiation and then characterize its resiliency through Raman spectroscopy, photo-current mapping and electrical characterization of the graphene field effect transistor. Detection of as few as 25 Si^+ ions is demonstrated at an energy of 20 MeV, with minor effects on the D^2GOS functionality. However, at lower energies, displacement damage occurring within the depletion region, does begin to show detrimental damage to the D^2GOS junction, resulting in increased dark charge generation. Raman spectroscopy does not show any damage to the graphene layer, only the underlying silicon absorber layer.

ORAL (INVITED)

Hierarchical Approaches to Scalable Nanomanufacturing of Thin Film Electronics

William Scheideler
Dartmouth College, Thayer School of Engineering

Electronics represents a largely untapped space for additive manufacturing, but opportunities for great economic and environmental impact abound. Applications in wireless sensing, robotics, and energy systems demand new solutions to seamless integration of electronics into flexible, stretchable, and 3D form factors. *Printed electronics* utilizing *nanomaterials* could potentially address this need for deeper integration and advanced functionality, but hierarchical approaches are, first, needed to bridge the length scales of *micro*electronics, *nano*materials, and miniaturized systems. These hierarchical approaches combine high-throughput, additive methods such as gravure printing with serial, direct write methods. This talk presents a framework for understanding how a combination of these methods can achieve scalable deposition and patterning while addressing limitations inherent to the physics of roll-based printing.

These hierarchical approaches also provide a route to extend nanomanufacturing to 3D structures. Lessons from planar printed electronics inform the material challenges of 3D integration, particularly those related to thermal and mechanical process limitations. Here we present strategies for nanomaterial ink design that can enable low-temperature integration of high-performance electronic materials and printed devices while leveraging multimodal energy inputs (UV, reactive species, etc). Finally, we evaluate the opportunities these strategies afford for applications in sensing and energy conversion.

ORAL (INVITED)

Aerosol jet printing of functionally graded materials

Ethan Secor, Rebecca R. Tafoya, Bryan J. Kaehr, Adam W. Cook
Advanced Materials Laboratory, Sandia National Laboratories, Albuquerque, NM, USA

In this presentation we introduce a multimaterial aerosol jet printing platform for on-the-fly mixing of functional inks, enabling digital printing of microscale patterns with non-binary control of material composition. This leverages advances in process understanding, custom printhead design, and software development to establish a versatile fabrication platform well-suited for functionally graded films. A fluorophore in an acrylic matrix provides a viable proof-of-concept demonstration to validate and characterize the technique. Extending this to functional materials, graded optical and magnetic thin film composites are shown. State-of-the-art capabilities and limitations of this fabrication platform will be discussed, along with compelling opportunities in functionally graded films and beyond. The development of a versatile multimaterial fabrication capability based on aerosol jet printing thus provides a promising platform to advance the scope of applications for digital printing.

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ORAL (INVITED)

Really Cool Molten Sodium Batteries: Material Innovations to Enable Low Temperature Operation

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Sandia National Laboratories, Albuquerque, NM USA

Though portable electronics and electric vehicles continue to benefit from new battery technology development, the safe, low-cost, reliable large scale batteries needed for grid-scale energy storage remain relatively undeveloped. Here, we describe a promising new class of molten sodium-halide batteries that show exciting potential as safe, cost-effective, long-lived batteries. These Na-NaI batteries utilize a solid state sodium ion conducting membrane to separate a molten sodium anode and a molten inorganic NaI-based halide salt catholyte. The molten salt catholyte not only promises a long cycle life, but offers a higher voltage (>3V) than traditional molten sodium batteries. Our goal is to engineer the materials chemistry of these new batteries to enable operation at temperatures near 100°C, a drastic reduction from the ~300°C common to traditional molten sodium technologies, while employing materials that avoid problems with thermal runaway and flammable electrolytes that often plague other battery technologies. Meeting this challenging objective requires creative engineering of materials and interfaces throughout the battery, and this presentation will highlight specific advances in molten catholyte composition and electrochemistry, the performance of solid state separators at these reduced temperatures, and the importance of liquid-separator interfaces in advancing the cycling behavior of assembled prototypes. Encouraging performance of these new "low" temperature molten salt batteries promises new opportunities to realize much-needed safe, reliable, and cost-effective large scale energy storage.

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ORAL (INVITED)

2D-Dirt: A Low Tech Material with High Tech Potential

Erik D. Spoerke,[1] Eric Schindelholz,[1] Kenneth Armijo,[1] Margaret Gordon,[1] Stephen Percival,1 Michael Melia, Derek Nelson, and Jaime Grunlan[2]
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2. Texas A&M University, College Station, TX, USA

Clays have been part of civilized culture for millennia as structural materials, water vessels, thermal coatings, decoration, and even food supplements. More recently, we have explored these natural 2D materials as elements of highly functional polymer clay nanocomposite (PCN) thin films, which have proven to be highly effective as gas barriers and flame retardants, only a few hundred nanometers thick. Here, I will describe a series of PCN thin films deposited using a Layer-by-Layer (LbL) process that takes advantage of the self-assembly of the constituent components, to create thin films composed of highly organized, alternating molecular layers of functional polymers and exfoliated clay platelets, commonly montmorillonite or vermiculite. While maintaining the resulting "brick and mortar" structure, by controlling clay selection, polymer matrix chemistry, and thin film microstructure it is possible to create highly functional and versatile thin film composites. Here, I will describe the synthesis and characterization of these materials and their potential utility addressing two modern technological challenges: 1) electrical arc fault mitigation and 2) corrosion inhibition, both applications where PCN thin films may impact the lifetime and safety of critical energy technologies.

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ORAL (INVITED)

Reliability of Components that Contain Brittle Materials

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All electronics used in society contain some type of ceramic material which is brittle in nature. These ceramic materials are often adhered to other materials resulting in stresses from CTE mismatch and thermal processing. The mechanical integrity of these brittle materials can have an impact on the functional performance of the component, which is of importance to high reliability applications such as the aerospace industry. Because ceramics fracture catastrophically and in a stochastic manner, it is difficult to assign a "strength" value to the material that would enable engineers to design a factor of safety around. This presentation will discuss the process in which one can attempt to quantify the reliability of a component. The topics of strength-size scaling and environmentally enhanced crack growth will be discussed. A soldered multi-layered ceramic capacitor will be used as an exemplar of how to implement these topics to determine the reliability of a brittle component.

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ORAL

Design of an in-situ single quantum emitter detection platform for the nano-Implanter

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Single photon sources (SPS) are of critical interest for a wide range of usages from metrology to the basis of quantum computation and sensing. SPS based on color centers in diamond and other wide band gap semiconductors such as hBN, SiC, etc. all require the control over both the x, y, z positioning as well as the number of optically active color centers. At SNL we have developed focused ion beam implantation using our nanoImplanter (nI) which allows for us to control the positioning to <50 nm and implant single impurity atoms using counted ion implantation. However, the conversion efficiency from implanted impurity atom to optically active color center can range from <3% to >80%. For the low efficiency processes we need to develop an in-situ technique to determine the creation of SPS. To ensure single color center formation we have designed an in-situ photoluminescence (PL) setup which will be directly integrated into the nI allowing for detection of single photon emission during ion implantation. This PL setup in conjunction with a Hanbury Brown Twiss (HBT) interferometer for detecting photon antibunching is an unambiguous indicator of single photon emitters. We will then be able to deterministically create and measure single defect centers in a range of materials systems with nanometer resolution.

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ORAL (INVITED)

Metal guided selective growth of 2D Metal Dichalcogenides

Vincent Tung[1,2], Lain-Jong (Lance) Li[1], Ming-Hui Chiu[1], Hao-Ling Tang[1]
1. King Abdullah University of Science and Technology
2. Lawrence Berkeley National Lab

2D transition metal dichalcogenide (TMD) layered materials are promising for future electronic and optoelectronic applications. The realization of large-area electronics and circuits strongly relies on wafer-scale, selective growth of quality 2D TMDs. Here, a scalable method, namely, metal guided selective growth (MGSG), is reported. The success of control over the transition-metal-precursor vapor pressure, the first concurrent growth of two dissimilar monolayer TMDs, is demonstrated in conjunction with lateral or vertical TMD heterojunctions at precisely desired locations over the entire wafer in a single chemical vapor deposition (VCD) process. Owing to the location selectivity, MGSG allows the growth of p- and n-type TMDs with spatial homogeneity and uniform electrical performance for circuit applications. As a demonstration, the first bottom-up complementary metaloxide-semiconductor inverter based on p-type WSe2 and n-type $MoSe_2$ is achieved, which exhibits a high and reproducible voltage gain of 23 with little dependence on position.

ORAL

Electronic and Structural Response of Rare-Earth Metal-Organic Frameworks with Acid Gases

Dayton Vogel, Dorina Sava Gallis, Tina Nenoff, Jessica Rimsza
Sandia National Laboratories, Albuquerque, NM, USA

Acid gases create harsh environments in which metal-organic framework (MOF) materials are known to degrade. Recent application of the rare earth (RE) MOF,[1,2] $RE_{12}(m_3\text{-}OH)_{16}(C_8O_6H_4)_{12}(C_8O_6H_5)_4$. (RE=Y, Eu, Tb, Yb) to acid gas separation has identified maintained crystallinity following exposure in a humid NOx environment, indicating possible application within NOx containing gas streams. Additionally, photoluminescent quenching following NOx exposure has been identified. To understand the possible quenching mechanisms, the optimized geometries, ground state electronic structures, and the resulting optical spectra have been calculated using density functional theory (DFT) simulations.[3] A comparison of geometric and electronic structures with adsorbed H_2O, SO_2, and NO_2 in various configurations highlight structure-property relationships between adsorbed acid gases in the RE-MOFs and provide insight into the reported stability and photoluminescent quenching.

1. Sava Gallis, *et al. ACS* Appl. Mater. Interfaces **2017,** *9*(27), 22268-22277.
2. Sava Gallis, *et al. CrystEngComm* **2018,** *20*(39), 5919-5924.
3. Vogel, *et al. Phys. Chem. Chem. Phys.* **2019,** submitted.

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ORAL

Electro-thermal Simulation and Performance Comparison of 1.2 kV, 10 A Vertical GaN MOSFETs

Luke Yates, Andrew Binder, Jeramy Dickerson, Greg Pickrell, Robert Kaplar
Sandia National Laboratories, Albuquerque, NM, USA

Presently, the only commercially available gallium nitride (GaN) based power switching transistors are lateral designs limited to 650 V rated blocking voltage. This limitation has primarily been due to the epitaxial growth of GaN on non-native substrates such as Si, which results in a high defect density, as well as the electric field distribution inherent in a lateral device layout. Further, reliability concerns based on the quality of the GaN material and the many interfaces in such devices have caused manufactures to de-rate device voltage capabilities significantly. While bulk GaN substrates remain quite expensive, their availability is increasing, and many groups are researching the development of fully vertical GaN transistors, similar to designs in more mature materials such as Si and SiC, to allow for much higher blocking voltage and power handling capability in a reduced form factor. Two types of MOSFETs that have been proposed for vertical GaN structures are the Double-well MOSFET (D-MOSFET) and the trench-gate MOSFET. In this work, we have performed electro-thermal simulations of both types of vertical structures using Silvaco ATLAS. Both devices are designed to handle up to 10 A with a blocking voltage of 1.2 kV. We first compare the thermal performance of each device while in DC operation at 10 A. The impact of the gate dielectric material on electrical/thermal performance and design is evaluated for SiO_2, Al_2O_3, AlN, and SiN. The reduction in electrical current for each device is explored as a function of the junction-to-case thermal resistance. Finally, the contribution of internal thermal resistances is evaluated to provide insight into potential device designs capable of achieving robust thermal performance while simultaneously maintaining high electrical performance.

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ORAL

Abnormal crystallization in glass-ceramic to metal seals

Rachel White, Zahra Ghanbari, Don Susan, Steve Dai, Brenton Elisberg, Sara Dickens
Sandia National Laboratories

Glass-ceramic to metal seals are compression seals commonly used in electrical contact pin assemblies. Recently, large lithium disilicate (Li2Si2O5) crystals have been observed in the glass-ceramic, which has led to further investigation of the glass-ceramic and precious metal pin microstructures and their interdiffusion. The large crystals were found to begin at the glass-ceramic to pin interface and extend hundreds of microns outward into the glass-ceramic seal. This increased fraction of Li2Si2O5, which has a different coefficient of thermal expansion (CTE) than the bulk glass-ceramic, results in a CTE mismatch within the glass and the development of tensile stresses through the sealing cycle. At the surface of the pin near the abnormal crystals, electron backscatter diffraction (EBSD) and energy dispersive x-ray spectroscopy (EDS) showed an unexpected body centered cubic (BCC) phase rich in P, Zn and Cu, indicative of substantial diffusion between the pin and glass-ceramic.

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ORAL (INVITED)

Multi-dimensional van der Waals heterostructures

Jinkyoung Yoo
Center for Integrated Nanotechnologies, Los Alamos National Laboratory

Emerging nanomaterials have attracted much attention due to their novel functionalities, but have also been hindered by lack of scalable synthesis and of ways of controlling characteristics. Atomically thin two-dimensional (2D) materials are good examples of novel materials set promising exotic properties and requiring established manufacturing approaches for practical applications. Heterostructuring is a powerful and general strategy to control physical properties of materials. Moreover, heterostructuring can offer novel characteristics differentiating the heterostructure from individual component in a structure. Recently, 2D/2D heterostructures prepared by stacking are being explored to observe quantum phenomena. However, fabrication of 2D/2D heterostructures has been limited by difficulty in preparation of individual 2D layers in controlled manner. Heterostructuring with 2D and conventional materials in other dimensions (e.g. bulk-like structure for 3D and nanowires for 1D) has shown great potential for multi-dimensional heterostructures. In this presentation I'll discuss how to prepare multi-dimensional heterostructures composed of 2D and conventional materials. The experimental approach is epitaxial growth Si, Ge, and ZnO on various 2D materials including graphene, hexagonal boron nitride, transition metal dichalcogenides. Absence of surface dangling bonds on a 2D material provides an unique opportunity to overcome materials compatibility issues. Nucleation strategy and novel characteristics of multi-dimensional heterostructures will be discussed in detail.

STUDENT ORAL COMPETITION

STUDENT ORAL

Permselective Separators for Grid Storage Alkaline Zn/MnO_2 Batteries

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Increasing awareness of climate change and the dangers of fossil fuels have spurred a need for faster integration of renewable energy sources onto the electrical grid. Rechargeable alkaline Zn/ MnO_2 batteries have emerged as a candidate to fill this need as they are low-cost, possess a high energy density, are environmentally inert and can be readily mass produced [1,2]. However, one of the technical hurdles is overcoming the limited cycle life, due to the formation of irreversible and resistive $ZnMn_2O_4$ and ZnO species on the cathode when zincate ($[Zn(OH)_4]^{2-}$) ions diffuse away from the anode and cross the battery separators [3].

In this presentation, we demonstrate the use of new permselective polymeric separators that can be used in higher depth of discharge Zn/MnO_2 batteries at faster rates. Several separators were screened for their zincate blocking abilities using our recently developed anodic stripping voltammetry methodology [4]. The polymeric separators were also tested for hydroxide diffusion where it is shown that they demonstrate selectivity for the monovalent hydroxide anion. Potentiostatic electrochemical impedance spectroscopy was used to measure the ionic conductivity of the separators which was found to be comparable with that of the commercial separators Celgard 3501 and Cellophane 350P00. A primary discharge of the full 2e- capacity of MnO_2 (617 mA h g^{-1}) was used to further test the ionic selectivity of the separator where the 2nd e- discharge plateau, indicative of the absence of zinc, was observed only for Zn/ MnO_2 batteries that utilized the selective polymeric separators.

[1] N. Ingale, et al., J. Power Sources 276 (2015) 7-18. [2] M. Kelly, et al., J. Electrochem Soc. 164 (2017) 3684-3691. [3] J. Gallaway, et al., J. Power Sources 321 (2016) 135-142. [4] J. Duay, et al., Electroanalysis 29 (2017) 2261-2267.

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STUDENT ORAL

Tuning Support Synthesis to Provide a Magnesium Aluminate Spinel Platform to Trap Thermally Stable Single Atoms of Platinum

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2. Chemical and Biological Engineering, University of New Mexico
3. Chemistry and Chemical Biology, University of New Mexico
4. Department of Chemistry, Technical University of Munich

Magnesium Aluminate spinel possesses many desirable properties for use as catalyst support, especially tolerance of high temperatures and reducing environments. However, this material was previously considered to be unable to trap single atoms of platinum, which limits its use as a fully regenerable, next generation catalyst support in reactions which require rapid regeneration, including alkane dehydrogenations. However, we have recently developed a novel spinel synthesis technique that generates a material which can trap high loadings of thermally stable single atoms of platinum. This synthesis is low temperature, environmentally benign, amenable to doping and highly scalable. These single atoms can be reversibly formed into nanoparticles in reducing environments and redispersed to single atoms under oxidation. As a test reaction, propane dehydrogenation is used to measure catalytic performance. Bare platinum on this spinel shows low activity, but this can be improved by the addition of 1st row transition metal dopants to the spinel structure.

STUDENT ORAL

Infrared absorption cross-section in SiNx thin films

Sara DiGregorio, Scott Habermehl
Sandia National Laboratories

In thin films, the magnitude of the infrared absorption can be related to the absorption cross section, σ. In this work, a composition-dependent σ was measured for the Si-N asymmetric stretch mode of SiNx films of varying composition and thickness. Thin films were deposited by low pressure chemical vapor deposition (LPCVD) at 850°C from mixtures of dichlorosilane and ammonia. For each film, σ was determined from Fourier Transform infrared spectroscopy and ellipsometric measurements. Increasing silicon content from 0% to 25% volume fraction amorphous silicon led to increased optical absorption and a corresponding systematic increase of σ from 4.77x10-20 cm2 to 6.95x10-20 cm2, which is consistent with a reported value of 4.83x10-20 cm2.1 We believe this trend is related to charge transfer induced structural changes in the basal SiNx tetrahedron as the volume fraction of amorphous silicon increases. Experimental σ values were used to calculate the effective dipole oscillating charge, q, for two films of varying composition. It was found that q increases with increasing amorphous silicon content indicating that compositional dependencies contribute to modulation in the Si-N dipole moment. Additionally, in the composition range investigated, we found that σ agrees favorably with trends observed in films deposited by plasma enhanced chemical vapor deposition.

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STUDENT ORAL

Investigating Anomalous Growth of Pt Particles during Accelerated Aging of Diesel Oxidation Catalysts

Deepak Kunwar, Abhaya Datye
Department of Chemical and Biological Engineering, University of New Mexico

When Pt catalysts are aged in air at 800 °C, we see significant growth of Pt particle sizes. The particle size distributions in the aged catalysts are usually bimodal, with some very large particles coexisting with smaller particles. Here we investigate the origins of these anomalous particle size distributions and relate them to the vapor phase transport of PtO_2 under oxidizing conditions. Our results suggest that the emission of PtO_2 from the catalyst into vapor phase could be a cause for the anomalous growth of Pt particles observed during high temperature aging. We show that supports such as ceria that can trap Pt ions cause a suppression of vapor phase transport, while the alumina and the $MgAl_2O_4$ spinel supports are unable to trap the Pt ions leading to the formation of abnormally large Pt particles.

STUDENT ORAL

Artificial Foliage with Remarkable Quantum Efficiency in Converting Photons to Formate

Hanqing Pan, Michael D. Heagy
New Mexico Institute of Mining and Technology

An apparent quantum efficiency (AQE) of 40% for the photo-reduction of bicarbonate to value-added formate was achieved by designing a novel thin film semiconductor device with metallophthalocyanines as the photosensitizer. The thin film device was fabricated by the thermal deposition of 100 nm of semiconductor (TiO_2 or Cu_2O) and 100 nm of zinc or cobalt phthalocyanine. We attribute these extraordinary results to the synergistic, foliated design of the positive hole scavenger and photosensitizer. The photo-excited phthalocyanines can transfer its electrons into the conduction band of the semiconductor, enhancing the overall electron supply. As demonstrated in this study, thin films in the form of artificial foliage are of high practical value because the immobilization of TiO_2 prevents agglomeration and maximizes surface area which allows for more bicarbonate adsorption and greater solar penetration. The ability to create the thin films via thermally depositing the photosensitizer and semiconductor allows for uniform layers without wasting material. Future studies include the use of transient absorption spectroscopy to confirm the mechanism of charge transfer from dye to semiconductor.

STUDENT ORAL

Reduction of Metal Acetylacetonates Utilizing Lithium Metal Hydrides

Paris C. Reuel, Timothy J. Boyle
Sandia National Laboratories

Copper has played an essential role in electronics for the past century. Its low electric resistance and cheap cost makes it a leading choice for wiring and circuitry; however, the metal easily corrodes and readily decomposes in radioactive environments (i.e., outer space, reactors). Substitutional alloys have long been used to improve the overall properties of metals by tailoring their properties (i.e., mailability, resistance, strength). In this study, we were exploring doping copper with alternative fcc-metals to increase its radiation stability (i.e., rad hard). To achieve this goal, a variety of nanometals were doped into copper nanomaterials and printed via ink jet processes. While routes to these nanometals, it was discovered a route in which a metal acetylacetonate ([M(acac)x]) when reacted with lithium aluminum hydride ([LiAlH4]) produced a mixed metal, aluminum nanomaterial. For this presentation, the synthesis of the [M(acac)x], characterization and properties of the products from the reduction of variety of [M(acac)x] by [LiAlH4] will be presented. In addition, the formation of nanoinks and the respective traces generated will be discussed.

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STUDENT ORAL

Nanoparticle Immunotherapy: A Novel Vaccine Platform

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Cancer immunotherapy is an important alternative to traditional treatments such as chemotherapy and radiation, oftentimes reducing the toxicity and negative side effects. Although immunosuppressive changes in the tumor microenvironment impairs normal immune surveillance against cancer in the body, eliciting an immune response for appropriate cancer antigens can be an effective approach for reactivating immune defense mechanisms and developing cancer treatments. Past studies have demonstrated the use of nanoparticles as delivery vehicles for various cargos. We have engineered immunogenic and biocompatible mesoporous silica nanoparticles that can carry several components in a nanoparticle core coated by a lipid shell. By loading the mesoporous core with the model antigen ovalbumin, which will be delivered to antigen-presenting cells (APCs), and incorporating the bacterial polyliposaccharide- derived monophosphoryl lipid-A (MPL-A) as an adjuvant to activate toll-like receptor 4 (TLR4) on APCs, we can elicit specific immune responses against the antigen. Via flow cytometry and confocal microscopy, results showed specific uptake of our immunogenic nanoparticles by APCs and other immune cells. In addition, the co-loading of MPL-A and ovalbumin proved to enhance antigen presentation and processing as well as APC activation. In vivo studies have also shown a heightened survival rate for mice treated with the co-loaded immunogenic nanoparticles. Based on these results, "nanoparticle immunotherapy" can stimulate cancer-specific immune responses and act as an effective cancer treatment.

UNDERGRADUATE POSTERS

UNDERGRADUATE POSTER

Probing Heterogeneous Polymer Chain Dynamics Near the Glass Transition: A Solid State 1H NMR Investigation

Joshua Allers, Brad H. Jones, Todd M. Alam
Sandia National Laboratories, Dept. of Organic Material Sciences

Thermosetting polymers play an important role in adhesive, coating and composite applications. In such polymers, the introduction of permanent chemical cross links leads to the formation of stresses during curing, thereby motivating fundamental studies directed at understanding and reducing residual cure stresses. It has been proposed that polymer systems with large heterogeneities can be fully cured at temperatures well below the final glass transition temperature (Tg). Here, we describe the use of solid state 1H nuclear magnetic resonance (NMR) spectroscopy to directly probe the polymer chain dynamics near Tg by utilizing dynamic averaging of the local 1H-1H NMR dipolar field. NMR then gives the polymer chain correlation times and activation energies (Ea) for the Tg process. Of specific interest is the impact dynamic heterogeneity has on the observed changes in the NMR line shape. By combining simulations and experiment, the line shapes were used to determine distributions in Ea for a series of thermosetting polymers with systematically varied heterogeneity.

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UNDERGRADUATE POSTER

Characteristics of Varistor Particle Lightning Arrestor Connector Breakdown

Samantha Andrews, Carolina A. Gomez, Pin Yang
Sandia National Laboratories

This study investigated the breakdown behavior in varistor based lightening arrestor connectors (VLACs) under different temperature and pressure conditions. A LAC must reliably pass operational signals, but fail in a permanently shorted manner when subject to high current from high voltage sources, such as lightning attacks and associated fire hazards, to protect critical components for high consequence electronic systems. Preliminary results obtained from a single pin tester under these conditions have shown a strong temperature dependence on breakdown behavior. This work studied the characteristics of VLAC breakdown, based on the waveforms collected from a single pin tester. Analysis on the variation of waveforms under different temperature and pressure conditions will shed light on the breakdown mechanisms for VLACs. Implications are important for weapon safety under normal and credible abnormal environments.

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UNDERGRADUATE POSTER

Self-Assembly of Porpyhrin Nanostructures

Ashley Bowman[2], Casey Karler[1], Michelle Upham[2], and Hongyou Fan[1,2,3]
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Porphyrins are a class of optically active biomacromolecular compounds which play critical roles in biological energetic processes including photosynthesis, and also serve as colorful pigments covering a wide range of the visible spectrum. In an effort to utilize these versatile porphyrins in advanced materials development, organized porphyrin nanostructures with photoactive properties have been obtained through a surfactant-assisted non-covalent self-assembly method (π-π interactions and ligand coordination) through the cooperative interactions of the porphyrin building blocks including zinc meso-tetra(4-pyridyl)porphine, tin meso-tetra(4-pyridyl)porphine, and meso-tetra(4-pyridyl)porphine. This method takes advantage of porphyrin insolubility when deprotonated in solution due to acid-base neutralization, thereby forcing them into surfactant micelles which stimulates self-assembly and eventually yields well-defined controllable external morphology. Electron microscopy characterization as well as X-ray diffraction confirmed controlled self-assembly of the macrocyclic building blocks into ordered nanostructures including nanorods, nanocubes, nanocylinders, nanooctahedron, nanowires and nanofibers. Investigation of variable parameters influencing the growth process showed that the final product morphology is determined by reaction conditions including pH, reaction time, injection speed, precursor concentration, and surfactant types. Optical characterizations using UV-Vis spectroscopy and fluorescence imaging and spectroscopy show enhanced collective optical properties over the individual chromophores, favorable for exciton formation and transport. With active and responsive optical properties, these porphyrin nanostructures look to serve as promising components for a wide range of practical applications including sensing, optics, nanoelectronics, diagnostics, solar cells, photocatalysis, and pollutant photodegradation.

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UNDERGRADUATE POSTER

Cathodic Reduction Kinetics on Stainless Steel Surfaces in Concentrated Magnesium Chloride Brines

Jacob Carpenter, Ryan Katona, Eric Shindelholz
Sandia National Laboratories, Albuquerque, NM, USA

Atmospheric corrosion, a process responsible for trillions of dollars a year in maintenance and safety considerations across many industries, is a process not fully understood in coastal environments. Marine sea salt aerosols adhere to surfaces exposed to marine environments and deliquesce forming a microscopic, aggressively corrosive electrolyte layer, especially in low RH where the electrolyte is primarily composed of magnesium chloride ($MgCl_2$). The electrochemical processes driving corrosion on these surfaces are studied here in the form of the cathode kinetics in $MgCl_2$ salt brines on 304L Stainless Steel (SS). A rotating disk electrode was used to simulate electrolyte films at various thicknesses in MgCl2 solutions corresponding to various equilibrium relative humidities. In $MgCl_2$ environments, the alkalizing effect of the cathodic processes caused the precipitation of $Mg(OH)_2$ buffering the surface pH much lower than similar environments. This caused the dominant cathodic reaction in saturated $MgCl_2$ to be hydrogen evolution reactions (HER) instead of oxygen reduction reaction. With enhanced HER kinetics, it is possible that an increase in stress corrosion cracking is present on the surface of SS alloys due to hydrogen embrittlement, causing an acceleration of part failure in marine atmospheric environments.

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UNDERGRADUATE POSTER

Influence of build orientation and surface finish on the corrosion of additively manufactured 316L

Jesse Duran [1], Michael Melia [1], Eric Schindelholz [1]
Sandia National Laboratories, Albuquerque, NM, USA

Metal additive manufacturing is unique in its ability to produce complex metallic parts. These complexities can cause microstructures and surface finishes which lead to large variability in surface properties like susceptibility to local corrosion. This study investigates how surface treatments and build orientation impact surface roughness and local corrosion initiation of 316L stainless steel parts using a powder bed fusion technique. Methods of surface treatment included grinding with SiC paper, tumble polishing, electropolishing, chemical passivation, and an in-process laser polish. To determine microstructural and tortuosity differences between the surface treatments and build orientations, cross-sections were analyzed using electron microscopy and electron backscattered diffraction. Surface roughness values (S_a and S_z) were determined using white light interferometry. The corrosion behavior was tested by anodic potentiodynamic measurements of the surface in a quiescent 0.6 M NaCl solution to determine a breakdown potential (E_b), an indication of pit susceptibility. In general, smaller S_a led to larger E_b,reaching maximums for the electropolished and ground surface treatments ranging on average from 0.95-1.22 $V_{Ag/AgCl}$ and 1.13-1.28 $V_{Ag/AgCl}$, respectively. The rougher and more tortuous surface finishes exhibited orientation dependent E_b values from 0.15-0.90 $V_{Ag/AgCl}$.

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UNDERGRADUATE POSTER

Gripping mechanisms for micro-scale optical fiber holders

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Design and optimization of optics and optical components is facilitated using digital manufacturing approaches such as 3D printing, enabling rapid prototyping and pre-alignment of components. For microscale optics, multiphoton lithography (MPL) is one of the only printing techniques that can achieve microscale (<1 µm) features with optical surface quality. In this work, we designed a micro-optic component that integrated a 200-micron diameter collimating lens with a pre-aligned fiber optic holder to accommodate a 125 µm wide fiber. Following initial studies to position the fiber in the holder, we realized the need for a mechanical gripping mechanism to accurately position and hold in place the fiber. Unlike common cable connectors that use clips, (set) screws, mated-indentions and other mechanisms to hold a cable in place, little work has been done to examine mechanical connectors at such a small scale. We prototyped four designs based on interior flaps and bow clips and examined both the fiber insertion force, placement and hold, and ability to remove the fiber. By varying the width, thickness and protrusion of the gripping mechanism into the fiber socket, our studies converged on a flexible bow clip design that showed good strength and repeatability. Overall this work—enabled via micro-scale rapid prototyping—offers a foundation to experimentally examine plug-socket type mechanisms that are orders of scale smaller than the ubiquitous device connections that pervade our daily lives.

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UNDERGRADUATE POSTER

Synthesis of fcc-Metal Precursors and Nanoparticles for Radiation Hard Electronics

Fernando Guerrero, Timothy J. Boyle, Thao H. Nguyen, Nathaniel Padilla, Xavier Robinson, Paris Reuel, Nelson S. Bell, Adam W. Cook
Sandia National Laboratories

The demand for higher efficiency and smaller electronics continues to grow. As such, the demand for a new generation of materials that can meet these needs also increases. Nanometals have come to the forefront in electronic applications due to ability to be printed and sintered at the required smaller dimensions. Of these metals, copper has been presented as a lower cost alternative to more expensive materials (i.e., silver and gold) and fine controlled printing of circuits has been realized. However, copper (and most metals) is susceptible to radiation damage, rendering them unusable in aerospace equipment, fighter jets, and weapon systems. In order to enhance the radiation stability of the nanoinks (N-inks) and develop radiation resistant printed materials, it was reasoned that doping copper with other metals may assist in stabilizing these materials to radiation damage. To accomplish this, nanocopper alloys were going to produced and tested for stability to radiation environments. In agreement with the face centered cubic (fcc) structure of copper, a variety of nano-fcc-metals including platinum, gold, silver, iron, cobalt, and bismuth were synthesized and used as dopants in a nanocopper ink. The syntheses, characterization, and ink formulations of the in situ and ex situ nanoalloys will be presented. Additionally, the printed traces were analyzed before and after ion irradiation to determine any impact radiation might have on these traces. The results from these studies will be presented.

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UNDERGRADUATE POSTER

Microstructure – Mechanical Strength Relationship of Aluminum Nitride

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Aluminum nitride (AlN) is a unique ceramic material due to its high thermal conductivity and electrically insulative properties. It is commonly used in the electronics industry as a heat sink where electrical conductivity is not desired. In high reliability applications it is necessary that the aluminum nitride be mechanically stable. Strength testing is a viable way to measure the spread of flaws in manufactured parts to determine their mechanical reliability. Biaxial flexure testing using a Ring-on-Ring fixture was used to test Sienna Technologies Inc. ST-200 AlN product. Results pointed to a bimodal strength distribution within the material. Microstructural characterization revealed that yttrium oxide (a commonly used sintering aid) had two types of dispersion within the aluminum nitride material: “vein-like” and “isolated particle” type structures. It was found that material machined near the surface of the aluminum nitride billet had the “vein-like” structure and material in the bulk had the “isolated particle” type structure. The “vein-like” structure resulted in lower strength material.

UNDERGRADUATE POSTER

Realizing rugged and conformable printed devices via In-Mold-Electronics

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2. Electrical and Computer Engineering, University of New Mexico, Albuquerque NM

In-mold electronics (IME) is an emerging technology whereby flexible conductive inks are printed onto moldable substrates. IME allows for the creation of circuits that are much thinner and lighter than traditional circuit boards, buttons, and wiring, with considerably more design freedom. The aim of this project was to create demonstrators to showcase IME capabilities at the Advanced Materials Lab (AML). We designed and successfully printed capacitive touch and near-field communication (NFC) demonstrator circuits. These circuits were printed using a direct-write machine and DuPont’s flexible conductive and dielectric inks onto polyethylene terephthalate glycol (PETG) or polycarbonate substrates, which were then thermoformed over various stereolithography (SLA) printed molds. Significant findings included considerable variation in dimension and resistance of traces with this printing method as well as a decrease in the resistance of traces after heat-curing or thermoforming. Of note, traces equal to or smaller than 400 µm wide and 30 µm tall were less likely to crack than larger traces. We are currently working on further characterization and troubleshooting for this method of creating IME at the AML, as well as additional demonstrators.

UNDERGRADUATE POSTER

Epitaxial PZT Thin Films on Low Dielectric Constant, Single Crystal Substrates

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3. Pennsylvania State University, State College, PA

Pyroelectrics are attractive for a variety of thermal detector applications due to their broad wavelength response and ability to operate without cooling. However commercial pyroelectrics-based detectors often fall ~>100x short of their predicted defectivity. Performance limits of thermal detectors are difficult to characterize because the mechanisms associated with domain switching occur in nanometer and picosecond resolution. Thus, in this work, we are utilizing Sandia's recently-developed Ultrafast Scanning Electron Microscope to enable microscale investigation of thermal and electrical excitation of PZT domains and elucidate the role of defects, strain, composition, and interfaces on the pyroelectric response. Epitaxial $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) on two substrates is demonstrated. First, epitaxial PZT on $SrRuO_3/SrTiO_3$ substrates were grown using pulsed laser deposition for thermal excitation experiments. X-ray diffraction data shows clear epitaxial orientation on the SRO/STO template and polarization hysteresis loops show clear saturation.

For electrical excitation experiments, substrates with low dielectric constants are required and growth of (100)-textured PZT thin films are demonstrated. As the first set of experiments, growth by chemical solution deposition was pursued to provide an opportunity in future experiments for rapid composition changes. The substrate mismatch between PZT (20/80) and MgO is ~6%; growth experiments to promote texturing across the large mismatch will be discussed. SEM images show 100-textured PZT grains with visible in-plan domain structure. X-ray diffraction (XRD) shows (100)-textured PZT grains. Influence of growth parameters on film orientation and microstructure will be discussed.

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UNDERGRADUATE POSTER

Materials Visually Responsive to Physical Stimuli

Jason Livesay, Matthew Humphries, Cody Corbin
Sandia National Laboratories

Materials that dramatically and irreversibly transform color upon physical damage are important for a variety of applications. These "bleeding" materials are akin to permanently bruised skin. A multidisciplinary team at Sandia National Laboratories has been developing a two-component material: a polymer in which a bi- or tridentate N-donor ligand is incorporated in the polymeric backbone combined with dispersed microspheres that encapsulate a transition
metal ion. Only the prior component will be discussed.

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UNDERGRADUATE POSTER

Study of antimony alkoxy carboxylates as dopants for zinc oxide varistors.

Nastassja Martin, Timothy J. Boyle

Sandia National Laboratories

Varistors are electrical components that have their electrical resistance adjusted by the voltage that is applied. These materials are often composed of zinc oxide that is doped with a variety of metals cations to further improve their properties. For our system, chlorides derivatives are currently used for the production of varistors. Exploring alternative systems has led us to investigate the use of carboxylic acid and alkoxide derivatives, due to their high solubility, low decomposition temperature, and ease of precipitation. One of the dopants that is of interest is antimony and antimony alkoxy (OR) carboxylates (ORc) are of interest because of the potential variability in steric bulk of the products that will allow us to control the final properties (i.e., morphology, particulate size, etc.). By varying the stoichiometry and steric bulk of the [Sb(OR)$_3$] and the H-ORc precursors, the reactions are expected to coordinate in a variety of different configurations. While there is little information available on antimony alkoxy carboxylates in the structure literature, other species have shown that the carboxylates can act as chelation, bridging, bridged chelation, and terminal configurations. A systematic investigation of a family of [Sr(OR)$_3$] (where OR = OCH_3, OCH_2CH_3, or $OCH(CH_3)_2$) modified by a series of sterically varied HORc (where ORc = O_2CH, O_2CCH_3, $O_2C(CH(CH_3)_2)$, $O_2C(C(CH_3)_3)$, or $O_2C(CH_2C(CH_3)_3)$) was undertaken to determine the various compounds that could be exploited for varistor applications. From these studies a novel structure, antimony diacetate mono-*iso*-propoxide ([$Sb(O_2CCH_3)_2(OCH(CH_3)_2$]) was isolated from the reaction of [$Sb(OCH(CH_3)_2)_3$] with H-O_2CCH_3, in a 1:3 molar ratio. Full characterization of this complex and additional results from this study will be presented.

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UNDERGRADUATE POSTER

Evaluating Surface Tension Self-Alignment of Flip Chip Bonded Die

Jessica McDow[2,1], Jaime McClain[1], Henry Dallo[1], Ian Young[1], Andrew Hollowell[1]
1. Sandia National Laboratories
2. New Mexico State University

Flip chip attachment processes are important for high I/O density devices and can increase interconnect density when compared to manual wire bonding. Solder die attachment like the IBM C4 process is used in a variety of MEMS and electronic microsystems and has an advantage with the ability to establish self-leveling and self-alignment due to surface tension forces. High precision die alignment is important for heterogenous integration development in particular for optic and photonic device integration, where unique constraints require sub-micron alignment accuracy. Flip chip die attachment is often done with two classes of bonding equipment; less expensive, lower precision pick and place tools have a +/- 10 µm accuracy where high cost, high precision flip chip bonders have a +/- 1 µm accuracy. In this work, we analyze two alignment techniques that take advantage of surface tension forces for die registration: 1. surface tension self-alignment due to confining the wettable metallization and 2. Mechanical registration between keyed structures of two chips placed on a single substrate. Post reflow alignment accuracies are presented on both of these approaches and this presentation will summarize the results of this investigation on whether we are able to match or outperform the high precision flip chip bonder and achieve a better than 1 µm alignment accuracy using a low cost pick and place tool.

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UNDERGRADUATE POSTER

Ultra-thin mesoporous silica-based membrane for high temperature hydrogen separation

Erick Metzner [1], Jimin Guo [1], Zane Armijo [1], Milan Rede [1], Ying-Bing Jiang [1], C. Jeffrey Brinker [1,2]
Department of Chemical and Biological Engineering, University of New Mexico

The recent discovery of more a than a 100-year supply of energy in shale gas in the United States demands efficient transformation of the hydrocarbon resources directly into value-added chemicals and fuels while maintaining a low environmental impact. Although various routes to synthesize olefin exist, production by dehydrogenation has been well-studied. However, developing an efficient conversion technology that is stable enough at high temperature to shift the equilibrium toward olefin production remains problematic. Here we describe a high temperature stable high flux membrane that is capable of continuously and selectively separating hydrogen from the reactor to promote the forward reaction. The membrane is based on a mesoporous silica film formed by evaporation induced self-assembly (EISA) followed by atomic layer deposition (ALD) and plasma processing. This is done to create a close-packed array of ultrathin hydrophilic nanopore channels in oriented anodisc pores, which support for further ALD deposition of Pd nanocrystals. The Pd nanocrystals inside the ultrathin hydrophilic nanopore creates a spanning Pd-based dense membrane that allows for perfect hydrogen selectivity. This ultrathin active Pd nanocrystals layer minimize the hydrogen diffusion distance that allows for high flux of hydrogen through the membrane.\

UNDERGRADUATE POSTER

The Synthesis of Barium and Strontium Oxides for Thin Films Production

Thao Nguyen, Timothy J. Boyle, Paul Clem
Sandia National Laboratories

Barium oxide (BaO) has been extensively used in electronic components research due to its high dielectric constant (BaO k = 37.4 at 300 K; SrO k = 14.6), high proton conductivity, optical and photoelectric properties. Due to these properties, BaO material is widely used in thin films, solar cells, and superconductor. The need for increasingly smaller electronic components parts requires thinner films but commercially produced BaO and SrO materials often contain additional unidentified chemical components, which are undesirable for film solutions. The current available precursors do not facilitate this process either, often forming carbonates that require much higher processing temperatures. Fluorinated precursors are often used to prevent carbonate formation. Here, the development of fluorinated alkoxide alkaline earth derivatives were undertaken to allow for the production of thin films of BaO and SrO. This was undertaken using barium (Ba^0) and strontium (Sr^0) metals, which were individually reacted with fluorinated ethanol ($H\text{-}OCH_2CF_3$; H-OEt-F) and fluorinated isopropanol ($H\text{-}OCH(CF_3)_2$; H-Pr^i-F) in a variety of organic solvents. Here we will report on the synthesis, the chemical structures, and other properties of these novel metal precursors synthesized. The conversion to BaO or Sro and the powder x-ray of the low temperature thin film produced will be discussed.

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UNDERGRADUATE POSTER
Synthesis of Indium Tin Oxide Films and Nanoparticles

Nathaniel Padilla, Timothy J. Boyle, Paul Clem
Sandia National Laboratories

The optoelectronic material indium tin oxide (ITO; $In_{0.74}Sn_{0.08}O_{2.0}$) has found widespread use in a wide number of applications. It was of interest to develop a route to transparent, conductive thin films of ITO for photovoltaic endeavors. Therefore, we undertook the synthesis of novel precursors to ensure a rapid, low-temperature, controllable stoichiometry for ITO thin films, using a series of metal amides, including: $[In(N(CH_3)_2)_3]$ and $[Sn(N(CH_3)_2)_2]$. The general synthesis consisted of dissolving the metal amide precursors in pyridine (~0.4M) and then dried to a powder *en vacuo* or spin-casted onto a substrate (platinized silica). Metal Amide precursors were characterized through TGA spectroscopy to identify temperature to burn precursors for bulk powders and anoparticle production routes. For the ITO compositions, Sn-rich s (97.0% Sn/3.00% In; 99.0% Sn/1.00% In; 99.9% Sn/0.100% In) and In-rich (97.0% In/3.00% Sn; 99.0% In/1.00%Sn; 99.9% In/ 0.100% Sn) powders and films were made and fully characterized. Bulk powders were then characterized through FTIR, PXRD, and XRF spectroscopy. XRF spectroscopy was vital in identifying low-percentage dopants.

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UNDERGRADUATE POSTER
Designer Depolymerizable Polymers Based on Ring-Closing Alkene Metathesis

Jackson Powers, Jeremy H. Herman, Brad H. Jones
Sandia National Laboratories

The depolymerization of polybutadiene by Ru carbenes is a highly efficient catalytic reaction that involves chain scission by ring-closing metathesis of fortuitously placed double bonds on the polymer chain. We hypothesize that linear and crosslinked polymers can be designed to be depolymerizable through introduction of moieties that exploit the same ring-closing mechanism. In this study, linear and crosslinked polyurethanes were prepared utilizing both commercially available and custom, unsaturated diols. Nuclear magnetic resonance spectroscopy was used to identify the formation of cyclic products indicative of a metathetic depolymerization upon introduction of Ru catalyst. Rheological measurements were performed in order to assess the corresponding effect of depolymerization on the mechanical properties of these polymers. Importantly, we found that a mixture of main-chain and side-chain double bonds in the polymer, ideally placed in a configuration enabling ring closure to cyclopentene or cyclohexene units, appears to be necessary for efficient depolymerization. Based on this finding, we designed a prototype rigid polyurethane foam that can be rapidly degraded upon exposure to Ru catalyst. This novel approach to depolymerizable polymers may provide a potential solution to the problematic permanency of polymers in a range of applications.

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UNDERGRADUATE POSTER

Lanthanide precursors and materials as surrogates for actinide-containing wastes.

Xavier Robinson, T.J. Boyle, J.A. Hubbard, F. Guerrero
Sandia National Laboratories

The obvious safety concerns associated with radioactive actinide (An = U and Th) waste has led to the exploration of lanthanide (Ln) based precursors and materials as surrogates. However, little work to verify the connection between this different family of compounds has been proffered. This effort focused on the development of nano-Ln oxide (LnOx) surrogates for pyrolyzed waste materials with verification by exploration of depleted uranium oxide (d-UOx) materials. Therefore, we explored both the synthesis, deposition, and pyrolysis behavior of both lanthanide oxide (Ln2O3) and actinide oxide (AnO2,) nanoparticles. Precursor to the LnOx and AnOx nanoparticles were synthesized from commercially available chloride (LnCl3, AnCl4), nitrate (Ln(NO3)3, AnO2(NO3)2), and acetate (Ln(OAc)3, An(OAc)4) salts. These were converted to nanomaterials through the introduction of common reducing agents (i.e., alkylamines and carboxylic acids) via solvothermal routes. The resultant nanoparticles were characterized by powder x-ray diffraction (PXRD), dynamic light scattering (DLS), and transmission electron microscopy (TEM). Lanthanide and actinide materials were then burned in a custom test chamber and the resulting flow and dispersion of particles was measured. A computer model was developed to determine a suitable lanthanide surrogate for future experimentation of waste conditions. Details of each aspect of this project will be presented.

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UNDERGRADUATE POSTER

Synthesis and characterization of tantalum precursors for the production of tantalum nanoparticles for radioactive shielding applications

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The use of tantalum in critical electrical component graded shielding has shown promise due to its high resistance to corrosion. Furthermore, the high Z nature of the metal makes it use of further interest. For this study it was of interest to add tantalum-based nanoparticles (Ta-NP) into a matrix for use as radioactive shielding. In order to achieve this goal, it is necessary to develop routes to Ta-based (i.e., oxides, metals, etc.) nanoparticles; however, the ubiquitous [$Ta(OEt)_5$] is limited in its utility due to its high reactivity. Controlling the hydrolysis and condensation of this precursor by modifying it with acids has been shown to be is critical in the final nanoparticle properties. To circumvent this in situ modification, the development of precursors that can readily convert to Ta-NP at a slower ore-controlled rate than the OEt derivatives was undertaken. Of these, the sterically bulky aryl alkoxides derivatives were of interest including, ortho-cresol(oMP), ortho-butylphenol(oBP), ortho-isopropyl phenol(oPP), 2,6-dimethylphenol (DMP), 2.6-di-*tert*-butylphenol (DBP), 2,6-diisopropylphenol(DIP). From these reactions of [$Ta(OEt)_5$] with HOAr, several precursors were structurally characterized as: [$(oMP)_4Ta(OEt)]_2$, [$Ta(oPP)_5(THF)$], [$(DIP)_3Ta(\mu\text{-}O)]_2$, [$(Cl)Ta(oMP)_4(THF)$], [$Ta(oMP)_5(HoMP)$], [$(DIP)_3Ta(O)]_2$. Nanomaterials syntheses for select species from this novel family of compounds along with [$Ta(N(CH_3)_2)_5$], $Ta(OC_2H_5)_5$, and $TaCl_5$ were undertaken to determine the impact the OAr derivatives have on the final nanomaterials compared to other precursors. Details of the synthesis, characterization and implementation of the various precursors and the subsequent nanomaterials will be presented.

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UNDERGRADUATE POSTER

Bio-Inspired Selective Ion Transport Membranes

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Membranes capable of selective ion transport are critical to technologies ranging from water purification to salt harvesting and even energy storage. Here, we describe a bioinspired approach to membrane synthesis that utilizes a commercial nanoporous, polycarbonate membrane substrate, treated with a layer-by-layer grown polyelectrolyte (LbL-PE) thin film coating. Our baseline PE film is a cation exchange membrane, containing alternately deposited layers of cationic polyethyleneimine (PEI) and anionic poly(acrylic acid). Chemical crosslinking is used to selective create an excess of carboxylic acids that facilitate selective cation transport. In addition to these baseline membranes, we evaluate the impact of additives, such as amino acids, believed to impact ion transport in biological ion channels. We specifically describe membrane synthesis and characterization, including evaluation of the ion selectivity of coated membranes. We show that select amino acid additions during LbL-PE synthesis can significantly impact ionic selectivity in these bio-inspired membrane constructs. Lessons learned from this work are expected to inform the development of cost-effective, scalable new ion transport membranes key to emerging ion-based technologies.

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UNDERGRADUATE POSTER

Metallization of Polymers via Cold Spray

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Cold spray is a thick film coating technology in which high pressure (10 bar-40 bar) pre-heated gas (100°C to 900°C) passes through a converging-diverging de Laval nozzle to achieve supersonic speed and acts as carrier stream for injected particles (typically metals). The kinetic energy of particles impacting a substrate drives plastic deformation and adherence to a substrate to produce dense, low-oxide coatings. The process is typically done on metallic substrates and is known for having a fast build rate and high deposition efficiency. Cold spray is an attractive process for the metallization of polymers due to its relatively low process temperature when compared to melt deposition processes. However, the high velocity of impacting particles and heating from the gas stream makes potential erosion and burning of the polymer substrate important considerations. In order to predict the temperature rise of the polymer substrate, first order calculations were conducted to estimate the kinetic energy transfer from particles to the substrate, and a basic gas dynamics model was used to generate a gas temperature profile in the nozzle. Experimental gas temperature measurements were performed to validate this model and showed that frictional heating may contribute substantially to substrate heating. Discrete particle tests were carried out to determine the effects of inlet gas temperature and pressure on particle embedment in various polymers. Further process optimization is necessary for a thick, well-adhered metallic coating to be achieved on a polymer substrate through cold spray. SAND2019-9620 A

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UNDERGRADUATE POSTER

Effects of Gap Filling, Surface Roughness, and Metal Work Function on LAC Breakdown Voltage

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This study investigated the effects of dielectric granule filling and work function on the fast rise breakdown (FRB) in lightning arrestor connectors (LACs). In the LAC, air gaps populated with PMN-PT (lead magnesium niobate-lead titanate) granules separate signal pins from a grounded web permitting reliable transmission of signals through the pins while safeguarding electronic systems by shunting unsafe high voltage, such as lightning, through dielectric-stimulated air breakdown across the air gaps. Therefore, the work function of the web including type of metal and surface roughness, as well as granule filling can play important roles on defining the maximum FRB voltage. This study used a specially designed testing cell, simulating a single pin, to study these factors on LAC breakdown. Results are important to the LAC design and fabrication for providing adequate safety margins for high consequence electronic systems.

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UNDERGRADUATE POSTER

Digital Fabrication of Compositionally-Graded Nanocomposites by Multimaterial Aerosol Jet Printing

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Advanced Materials Laboratory, Sandia National Laboratories

Aerosol jet printing offers a digital, non-contact, high-resolution direct-write capability with broad materials versatility. In this work, a multimaterial aerosol jet printhead is demonstrated for in-line mixing of multiple functional inks. Combining advances in custom printhead design and software tools, this enables direct patterning of compositionally-graded films. A proof-of-concept experiment using a fluorescent tracer validates this approach and allows straightforward visualization and characterization. In this case, composition information is obtained from fluorescence microscopy and profilometry measurements to calibrate deposition parameters and assess print quality. This on-the-fly mixing method provides a rapid, digital, and low-waste method to control print composition, which is extended to graded optical and magnetic nanocomposites to highlight the diverse and promising applications for this technology.

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UNDERGRADUATE POSTER

Relating Build Parameters, Density, and Structural Properties in Additively Manufactured 316L Stainless Steel

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Sandia National Laboratories, Albuquerque, NM, USA

This project investigates the Thermal Energy Density (TED) values in additively manufactured (AM) 316L stainless steel and how they affect the structural material behavior. TED is a measure of heat distribution during the build determined from thermal imaging data. TED values were measured during the build process by Sigma Labs for each of the different build plates and samples. Charpy impact toughness was measured through Charpy testing. Porosity was measured through Archimedes density principal. Microstructural information such as porosity was also obtained at SNL. Through examining the relationship between TED, density, and Charpy toughness we hope to identify a trend between TED and the build plate parameters. We hope to inform multiscale models to improve structural integrity through improved prediction of microstructure-property relationships. Additionally, several sizes of tensile bars were printed to identify the impact of TED on the unloading modulus, ultimate tensile strength, and yield stress. Mechanical properties of the tensile samples such as unloading modulus, UTS, and yield stress were collected using High Throughput Tensile testing at SNL. It was found that Structural properties could be predicted by TED in 316SS due to the ability of TED to predict porosity in this low power regime.

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UNDERGRADUATE POSTER

Microwave synthesis of oxidation-resistant copper nanoparticles for additive manufacturing applications

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Additive Manufacturing (AM) processes such as aerosol/ink-jet printing are non-contact deposition methods that can be used to deliver functional nanoparticle-based inks for the fabrication of electronic components such as resistors, transistors, and capacitors. As AM processes continue to expand, the development of reliable and versatile nanoparticle-based inks is critical. Copper nanoparticles (Cu NPs) have garnered attention due to their high electrical and thermal conductivity, high melting point, and relatively low cost compared to other metals (i.e., gold and silver). Despite numerous published synthetic routes to generate Cu NPs, the issue of inhibiting oxidation and corrosion, has been difficult to achieve, especially via green synthesis routes using minimal reaction times. The majority of the published routes involve harmful (toxic) compounds and reducing agents, as well as very high temperatures/long reaction times. For this project, we have explored microwave synthetic routes, using an in-house precursor (copper-mesityl) and a variety of green solvents (glycols) and surfactants (amines). Numerous synthetic parameters (i.e., solvent type, precursor concentration, and temperature) were systematically investigated to evaluate their effect on the final product. The high-quality nanoparticles were subjected to a wide variety of oxidation tests to analyze the role of the solvent and surfactant species have in hindering oxidation, as well in the presence of H_2S gas. Particles were characterized with PXRD, TEM, FTIR, and XPS. Details on the synthesis route, characterization, oxidation stability, and printing behavior are presented.

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GRADUATE POSTERS

GRADUATE POSTER

IN-SITU PRESSURE MONITORING OF DUAL-CURE THERMOSET RESINS FOR DIRECT-INK WRITING

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Direct-ink write is a type of additive manufacturing where a resin is extruded into filaments to build a structure in a layer-by-layer manner. Traditional resins consist of ceramic or metal-particle loaded binders, but recent research has investigated printing thermoset polymers. One approach to printing thermosets is by using dual-cure resins. Dual-cure thermoset resins consist of a photo-curable component and a thermally-curable component, where the photo-curable component is cured while printing to lock-in the structure, then the part is thermally cured post-print to achieve the ultimate mechanical properties. The viscosities and rheology of different resin formulations can differ significantly depending on the resin and filler types, and different printer parameters such as UV light intensity, print pressure, pump ratio, and print speed may be required to print different formulations. Changes in resin types and print parameters can require laborious re-optimization to obtain high quality final parts. One approach to reduce the time needed for process optimization is the development of in-situ process monitoring. In-situ process monitoring can be used to more rapidly optimize print parameters during a single print session or to identify changes in properties and flag a process issue such as clogging due to fillers or UV cure propagation up the print tip. This work explores the application of in-situ pressure monitoring as a process control for dual-cure thermoset resin used in DIW printing.

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GRADUATE POSTER

The Endocytotic Fate of a Mesoporous Silica Nanoparticle Supported Lipid Bilayer CRISPR Delivery Vehicle

Angelea Maestas-Olguin[1], Achraf Noureddine[1], Annette Labauve[1], Edwin Saada[1], Kimberly Butler[2], Oscar Negrete[2], Rita Serda[1,3], Jeffrey Brinker[1]

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CRISPR gene editing technology is strategically foreseen to control diseases by correcting underlying aberrant genetic sequences. In order to overcome drawbacks associated with AAV-CRISPR, the establishment of an effective non-viral CRISPR delivery vehicle has become a primary goal for nanomaterial scientists. Herein, we introduce the first monosized lipid-coated mesoporous silica nanoparticle (LC-MSN) delivery vehicle that enables loading of CRISPR components (11% *wt* RNP) with efficient release within cancer cells (~70%). With a low toxicity and a clathrin-mediated endocytotic internalization pathway, the gene editing efficiency in a reporter cell line was up to 10% using ribonucleoprotein (RNP) complex (Cas9/gRNA) and a CRISPR plasmid. The structural and chemical versatility of the silica core and the lipid coat along with their biocompatibility make LC-MSN a promising vector towards safe CRISPR components delivery and enhanced gene editing.

GRADUATE POSTER

Development of ceramics for electrochemical oxidative coupling of methane

Shanti Nayak, Angelica Benavidez, Lok-kun Tsui, Fernando Garzon
Center for Microengineered Materials (CMEM), University of New Mexico

Natural gas serves as an excellent bridge fuel as we transition to a low carbon economy. However, the high C-H bond strength and the directionality of the sp3 orbital in the methane molecule make it difficult for methane to form bonds with other species or catalytic surfaces. Hence, high temperatures and effective catalysts are required to activate and transform methane into useful chemicals, products, or electricity. [1] Tuning catalytic activity by electrochemical methods provides enhanced control of catalyst redox state and nanocatalyst activity. The presence of an electrical potential can dramatically alter the energy profile of the chemical reaction by lowering the activation barrier for the forward reaction. [1] The oxygen content of non-stoichiometric oxide catalysts can be controlled electrochemically, thus altering catalytic activity. We are developing electrochemical micro reactors to investigate oxidative coupling of methane reactions with better selectivity. By designing cell capacitance and resistivity, the reactor can be switched at high rates and this may change the methane conversion selectivity. The micro reactors are composed of ceria, lanthanum manganite and YSZ and are fabricated using ceramic additive manufacturing. Experiments involve the study of the thermodynamic stability and redox behavior of our printed materials using high temperature cyclic voltammetry techniques, heterogeneous conversion of methane to CO using our printed La(M)MnOx as catalysts and printing and characterization of ceria and rare earth doped ceria films as the electrolyte/catalyst support.

[1] Gür, T. M. Energy Combust. Sci. 2016, 54, 1–64.

GRADUATE POSTER

Simulations of dislocation interaction with free surfaces

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Simulation of dislocation dynamics for materials under loading is always a challenge especially when the computational volume is finite. Analytic solutions for a dislocation stress field need to be adjusted by adding a correction term to meet physical boundary conditions on a free surface. This correction term can be calculated using collocation points with a distribution of dislocation loops on the free surface(s). In our current research, we have developed a generalized method to find the Burgers vectors for surface loops of different shapes (i.e. rectangular, triangular) which nullify the stress traction on the surfaces at the collocation points.

PROFESSIONAL POSTERS

PROFESSIONAL POSTER

Strength Testing of Ferrite E-Cores: Manufacturer Comparison

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Ferrite is a ceramic material made from iron oxide and small quantities of other metallic elements. This creates an electrical insulator that is ferrimagnetic. Mn-Zn ferrites are commonly used as cores within high frequency transformers since they can easily change their magnetization. The lifetime of a component is greatly influenced by the mechanical properties of the core, as it drives the desired qualities of the part. Investigating and understanding the mechanical behavior of E-shaped ferrite cores, like those used in PulseR transformers, is necessary to ensure high reliability parts. A 3-point-bend test was performed on sets of cores from two manufacturers (Tomita and ACME). The cores were also tested in two orientations to investigate different stress concentrations within the parts. Data from the testing showed significant differences between testing orientations and manufacturers, with the ACME cores breaking at higher loads. Modeling of the parts was used to determine the maximum principle stress in each orientation, which confirmed the fracture data observation that ACME cores sustained higher stresses before breaking. Microstructural characterization was used to correlate material defects with differences in strength performance.

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PROFESSIONAL POSTER

Coloumbic Friction in Metamaterials to Dissipate Mechanical Energy

Zachary Casias, Anthony Garland, Katarina Adstedt, William Mook, Bryan Kaehr, Bradley Jared, Brian Lester, Nicholas Leathe, Eric Schwaller, Brad Boyce
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A metamaterial is comprised of unique unit cells that form a coherent structure or lattice (also known as architected materials, micro-trusses, and periodic cellular structures). In recent years, metamaterials have emerged as a promising solution for delivering novel material properties unattainable in monolithic materials such as high strength to weight ratio, increased damage tolerance, high energy absorption, and negative Poisson's ratio. For certain materials, adding a friction element to the unit cells enables these metamaterials to dissipate up to three times more mechanical energy than the material can store elastically. This simple approach of changing the function, the architecture, and the material of the unit cells enables the design of metamaterials with tailorable material properties. In this work we examine frictional effects of a variety of metamaterials with varying sizes, materials, and temperatures.

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PROFESSIOJNAL POSTER

Wetting behavior of glass-ceramic on stainless steel under different atmospheric and surface conditions

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The strength of glass-ceramic to metal seals can be heavily affected by the chemistry of the interface between the glass-ceramic and the metal. The wetting angle between the glass-ceramic and the metal can be a good indicator of final bond strength. In this study, the wetting behavior of a lithium-alumino-silicate glass-ceramic on stainless-steel was studied under different atmospheric and metal surface conditions. Experiments were run under nitrogen and argon environments with as received, vacuum baked, and pre-oxidized metal. A glass cylinder was placed on a stainless-steel plate in a tube furnace such that the cylinder was backlit, and a camera was used to capture the silhouette. The samples were heated above 1000C and images were routinely captured during the flow and the wetting of glass-ceramic on the metal surface. Dependence of wetting angle on stainless steel surface conditions under different environments will be presented and discussed.

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PROFESSIONAL POSTER

Direct write waveguides using multiphoton lithography

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Abilities to capture, guide, and direct light into pixelated detectors (CCDs, CMOS sensors, FPAs, etc.) using free-form trajectories would be transformative for a range of technologies that currently use traditional optics (lenses, mirrors, prisms, etc.) for light coupling. However, few manufacturing techniques provide the appropriate scale and surface quality to address this task. In this work, we consider "free-form waveguides" using the high-resolution 3D printing technique of multiphoton lithography (MPL; also known as direct laser writing, DLW). First, we printed hollow and solid core vertical waveguide arrays spanning millimeters with single (5 micron) and multimode (30 micron) compatible cross-sections. Unsupported 5-micron diameter pillars generally succumbed to capillary forces during development and drying and thus sheathed waveguides were designed by anchoring fibers to a support scaffold. In addition, we examined direct printing onto active devices (coupling a source to a sensor) using an air-clad multimode design. Efficient light coupling was observed with scattering losses primarily from fabrication artifacts such as stitch lines. To address these issues, we considered stitch-free cores using a clad-only design resulting in encapsulated photoresist in the interior that is subsequently cured (UV, thermal) following development. These initial results, combined with the limitless design space afforded the MPL technique, provide a promising path forward to develop ultra-wide-field and highly compact imaging devices.

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PROFESSIONAL POSTER

Laser weld hot cracking behavior of austenitic stainless steel with boron microalloying additions

Alex Hickman, Jeffrey M. Rodelas
Sandia National Laboratories

prevent hot cracking of laser welds, stringent control of base material alloy chemistry is necessary. In the case of controlled chemistry 304L, relatively small (~20 wt. ppm) boron addition has been shown to produce a distribution of chromium-rich borides co-located in delta-ferrite stringers. Previous work found that in as-received material, concentrations of boron up to 20 wt. ppm boron indicated no risk of heat affected zone (HAZ) liquation crack susceptibility. However, recent work has found that for similar boron concentrations, HAZ cracking can occur during laser welding if the distribution of chromium borides changes as the result of high temperature (>1000°C) thermal processing steps. This led to an in-depth investigation of several time-temperature combinations in order to determine potential impacts on weldability behavior and the risk of HAZ liquation cracking due to microalloying additions of boron. Light optical microscopy of etched laser welds on 304L was used to characterize the effects of various time-temperature combinations on changes to chromium boride distribution. The results of this analysis will be used to define acceptable part thermal processing conditions to avoid hot cracking of 304L laser welds.

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PROFESSIONAL POSTER

Extrusion of unilamellar lipid nanotubes by kinesin-powered microtubule filaments

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Cytoskeletal filaments and motor proteins are involved in organelle transportation and reorganization in eukaryotic cells.Previous studies demonstrated the ability to recapitulate the microtubule-kinesin transport system *ex vivo* to fabricate large-scale nanotube networks from multilamellar liposomes and polymersomes. Specifically, surface-absorbed kinesin motors drive biotinylated microtubules that interact with biotinylated vesicles via a streptavidin bridge, extruding lipid nanotubes (LNTs) from these vesicles and generating millimeter-sized branched networks. It is unknown, however, if such networks can be generated from giant unilamellar vesicles (GUVs), and if so, whether the lipid composition can be tuned to alter the dynamics, structure, and fluidity of LNT networks. Here we demonstrate that LNTs can be fabricated from GUVs in a two-step process where microtubule motility (*i*) drives transport and aggregation of GUVs to form structures with a decreased energy barrier for nanotube formation, and (*ii*) extrudes LNTs without destroying parent GUVs. We further show that the lipid composition of the GUV influences LNT formation. For example, GUVs primarily composed of liquid-disordered phase lipids readily formed highly branched LNT networks. Furthermore, phase-separated GUVs (e.g., liquid-solid phase-separated, and coexisting liquid-ordered and liquid-disordered phase-separated) also formed LNTs, where the specific phase behavior was reflected in the morphological properties of the LNTs. These results collectively demonstrate that membrane fluidity is vital to the formation and characteristics of LNTs. Overall, the ability to form nanotubes from compositionally complex vesicles opens the door to generating lipid networks that more closely mimic the structure and function of those found in cellular systems.

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PROFESSIONAL POSTER

Characterization of commercial ceramic cements as a binder for thermopile fabrication

Aaron D. Melad, Jon Height, June Stanley, Monique Curley and C. Ramesh Koripella
Sandia National Labs

A thermopile consists of several P-type and N-type thermoelectric couples connected in series, parallel, or series-parallel combination depending on the voltage and power output requirements. If the aspect ratio of a thermopile and the cross-sectional area of the individual legs is small, then a binder is required to provide structural rigidity to hold together all the thermoelectric elements into a thermopile. Depending on the operating temperature of the thermopile, organic polymer binders may not be suitable, and a high-temperature stable inorganic binder is needed. Ceramic cements are ideally suited for binder application because they are typically cured at low temperatures and they offer exceptional thermal stability to very high temperatures. Low temperature curing of ceramic cements avoids the potentially adverse reactions between the binder and the thermoelectric elements, which is a major concern with typical glass binders. In this work, several commercial ceramic cements, selected upon their low thermal conductivity and matching coefficient of thermal expansion, were evaluated for binder applications by characterizing their adhesive strength properties with bismuth-telluride based thermoelectric elements. Consistent size test coupons were prepared, and a test procedure was developed to perform pull strength tests in tensile mode. The effect of different surface preparation procedures of BiTe tiles, such as etching, polishing, and mechanical abrasion were also studied. Based on these studies a few suitable cements were down selected for further characterization work in thermopile application. Using one of the promising cements, a simple 2x2 array was fabricated and tested.

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PROFESSIONAL POSTER

Electrochemical Nitrogen Reduction on Exfoliated MXene ($Ti_3C_2T_x$)

James Park, Stanley S. Chou
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Electrochemical nitrogen reduction has been an emerging field to provide a benign method for ammonia production in comparison to the Haber-Bosch process which requires high temperature and pressure. In addition to the numerous publications on different materials that can electrochemically produce ammonia, several articles have also been published emphasizing the importance to carefully characterize the produced ammonia as background ammonia can be a significant source of error. Here, we investigate electrochemical nitrogen reduction on MXene ($Ti_3C_2T_x$) nanosheets that was recently reported to produce ammonia at low overpotential with faradaic efficiency of ~5%.[1] By developing a fundamental understanding of the catalytic activity of MXene, the performance can be improved and provide insight for further catalyst development. Moreover, other MXenes with different chemical components can be explored to study the effect of chemical composition on the catalytic activity.

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PROFESSIONAL POSTER

Ceramic Sodium Ion-Conducting Separator Processing

Amanda Peretti, Eric Coker, Mark Rodriguez, Martha Gross, Erik D. Spoerke
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Sodium-based batteries stand to become an important part of emerging large scale electrical energy storage infrastructure, utilizing domestically abundant sodium and promising improved safety, cost, and battery lifetime, relative to existing grid-scale batteries. Central to battery lifetime and performance of these batteries is a robust, highly conductive solid state separator that mediates selective sodium ion transport between the anode and cathode during battery cycling. NaSICONs ($Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ $0<x<3$) are particularly promising candidate ceramic ion conductors, with reported conductivities greater than 1mS/cm at room temperature. These materials are, however, notoriously difficult to synthesize on large scale with high phase purity and density, two properties that significantly affect their performance. Here, we describe the use of scanning thermal analyses and variable temperature x-ray diffraction to understand and direct the solid state synthesis of NaSICON from simple reagents. These studies not only inform conditions for reactive sintering of NaSICON ceramics, but also how the addition of excess volatile species and the impact of hydrate formation can impact ceramic properties. Insights from this work has led to the utilization of these ceramics in functional prototype sodium batteries currently in development.

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PROFESSIONAL POSTER

Solder Cup Wire Insertion Study

Shelley Williams
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Should 100% wire insertion remain a requirement for soldering during cable fabrication? Three conditions are required by the Association Connecting Electronic Industries for an acceptable solder cup connection (IPC-A-610): Wire leads must contact back wall of cup, be inserted for the full depth of cup, and visible solder must vertically fill at least 75% of the visible cup. Recent use of X-ray micro computed tomography (uCT) scans have revealed that solder cups can appear to be 100% filled and wires fully inserted but contain significant voiding at the bottoms of cups. To establish a technical basis for continuing the 100% insertion requirement and ascertain how best to measure it, solder joints from connectors were examined via uCT and joints were pull tested to correlate wire insertion, solder fill, and joint angle with joint strength.

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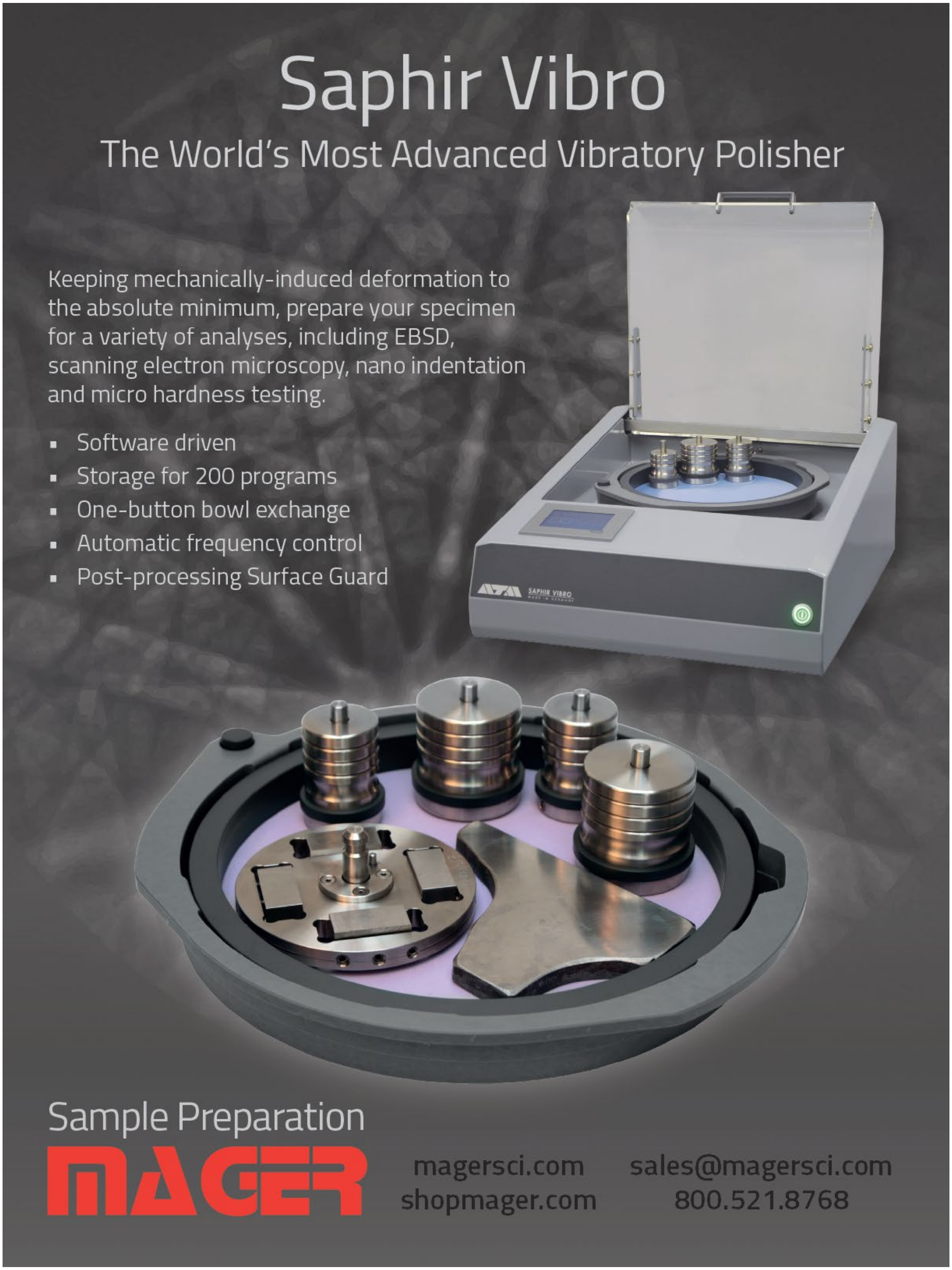
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