Livermore, CA 94550). Biological hazards and chemical hazards are commonly found within the same project at Lawrence Livermore National Laboratory (LLNL), however no established system currently exists to do a comparative analysis of the degree of implementation of safety controls for both types of hazards. A Laboratory Assessment Worksheet was created to devise a way to quantitatively compare the hazards, controls, and the degree of risk management actually present. Four numerical values—a biological hazard score, a chemical hazard score, a biological control score, and a chemical control score—were calculated to accomplish the comparison. The worksheet utilizes the Centers for Disease Control and Prevention's biosafety levels as a score for biological hazards; Sax's Dangerous Properties of Industrial Materials hazard ranking in combination with an exposure potential evaluation for the chemical score; and a percentage of a standardized list of controls for the control scores for both hazards. Once scores for each of the four categories are tabulated, the ratio of the hazard score to the control score can be used to decide whether the controls are appropriate for the particular hazard, i.e., the degree of risk management. Upon further development this worksheet will become a unique tool for the Hazards Control Department at LLNL because it will serve as an initial screening tool with the ability to compare biological and chemical hazards in a single experiment as well as biological and chemical hazards across multiple experiments.

Material Sciences

A Novel Approach to Estimating Thermal Conductivity. *GORDON WU (University of California–Berkeley, Berkeley, CA 94720) TIM KNEAFSEY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* Scientists at Lawrence Berkeley National Laboratory (LBNL) are currently researching natural gas recovery from gas hydrates in hopes that this will one day become a viable source of energy. Natural gas hydrates are water crystals located below permafrost and submarine environments that contain methane gas. Knowledge of heat flow through the hydrate-bearing reservoir must be understood and thermal conductivity is a fundamental property of a material that indicates its ability to conduct heat. The technique for estimating thermal conductivity calls for applying a temperature changes and using thermocouples to accurately measure the rate of temperature change. The thermal data were analyzed using Microsoft Excel and iTOUGH2. The program iTOUGH2 computes a best-fit to our measured data by optimizing the thermal conductivity through automatic model calibration. ITOUGH2 estimates the thermal conductivity based on previous output values and given parameters. The four materials used were dry sand, polyvinyl chloride (PVC), high density polyethylene (HDPE) and Pyrex borosilicate glass, and were chosen because they have thermal conductivities close to that of hydrate bearing sand (2.7 W/m K). Good matches were obtained between the simulations and the measured data showing the validity of the technique. It is important to realize that the substances that we were using can vary in thermal conductivity depending on the temperature, the porosity of the particular substance, and the composition of the sample. Now that the technique is validated, it can be used in other experiments to measure thermal conductivities.

Atomic Layer Deposition of Tin (IV) Oxide and Indium Tin Oxide Using Tetrakis(Dimethylamino)Tin Precursor. *DAVID BAKER (University of Illinois at Urbana Champaign, Urbana, IL 61802) GREGORY KRUMDICK (Argonne National Laboratory, Argonne, IL 60439).* Thin films of tin oxide were deposited on silicon wafers (001) and glass by Atomic Layer Deposition (ALD) using alternating pulses of Tetrakis(Dimethylamino)Tin and an oxidizing precursor. Doping tin oxide films with various reagents, such as indium, can create smooth, optically transparent and conductive coatings with applications in solar cell, gas sensor, and flat panel display technologies. Using deposition temperatures between 100–400°C, and exposure times ranging from 0.5 to 8 seconds, growth of a film was evident on Al2O3 coated substrates. For the silicon and glass substrates, measurements from the spectroscopic ellipsometer showed the thickness of the film increased with temperature and increased linearly with the number of cycles (maximum of 1.5 Å per cycle) during the ALD growth. At lower temperatures, extending the exposure times of each precursor demonstrated a self-limiting reaction. Growth at higher temperatures did not demonstrate a self-limiting reaction. This precursor was also used to create Indium Tin Oxide (ITO) films also by ALD. As evident from 4-point probe resistivity measurements, tin oxide and ITO films are excellent conductors with good optical transmittance. Characterization of the films was furthered by x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), x-ray florescence (XRF), and scanning electron microscope (SEM). Tetrakis(Dimethylamino) tin precursor demonstrated consistent ALD growth on glass and silicon surfaces coated with Al_2O_3.

Characterization of Nano-Particles in Mesophase Pitch Derived Graphite Foams. *JENNIFER MUELLER (Virginia Polytechnic Institute and State University, Blacksburg, VA 24060) JAMES KLETT (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* The addition of nano-particles to a raw material can significantly alter the structure and therefore properties of a material. A characterization study was conducted to explore the effects of nano-particle additions on graphite foam, a material that exhibits very high thermal conductivity and low density. Carbon nano-particles were added to mesophase pitch in varying amounts and processed to create graphite foam. Image analysis was conducted on each sample by using an optical microscope, Scanning Electron Microscope (SEM), and Transmission Electron Microscope (TEM). Other analyses included density measurements, compression tests, permeability tests, and flash diffusivity tests. Results showed that there were overall trends of decreasing density, thermal conductivity, and strength with an increasing amount of carbon nano-particles, but the permeability increased. Through optical image analysis, it was determined that the ligament size of the graphitic matrix decreased and that there was a significant disruption of graphitic plane alignment with greater additions of carbon nano-particles. Additionally, it was seen with the SEM that the number and size of open pores increased with an increasing amount of carbon nano-particles. Overall, the decreased ligament size and disruption of graphitic alignment explains the decreased strength and thermal conductivity, respectively. Also, the addition of the nano-particles increased the open porosity and, therefore, increased the permeability of the foam. As a result, the graphite foams characterized through this study are suitable for applications where higher permeability foams are desired. Since the mixture with the greatest amount of nano-particles had the highest permeability, a further study should be conducted to determine what mixture results in the maximum permeability of the graphite foam without a significant loss in thermal and mechanical properties.

Characterization of Sub-diffusion within Benard-Rayleigh Advective Cells by Examination of a Velocity Field with Additive Noise. *MARSHA LAROSEE (University of Michigan, Dearborn, MI 48128) BEN CARRERAS (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* Normal diffusion worked out by Einstein and Taylor is modeled by averaged particle 'Brownian motion' such that a given particle's motion is determined by *random* collisions with surrounding particles. Less well understood is the subject of anomalous diffusion, which is studied in many fields where diffusion influences the system (e.g., heat, fluids, chemical kinetics). The distinction between normal diffusion, a random mechanism and anomalous diffusion, that is a mixture of *random* and *deterministic* processes, is the time scale at which the transport occurs. Both diffusion and anomalous diffusion follow a power law relation $< \Delta r\ s > 1/s \approx t\ q(s)$, where $q(s) = 1/2$, $< 1/2$, $> 1/2$ for diffusion, sub-diffusion, and super-diffusion. Thus, sub-diffusion and super-diffusion scale with time differently than random motion predicts. In order to study sub-diffusion a deterministic model must be used while adding randomness, or noise to the system. A model referred to as the random walk with pauses or trapping events was investigated in order to characterize sub-diffusion in a fluid system. The system that was studied is an array of Benard Rayleigh advective cells where the velocity fields cause 10,000 tracer particles to circulate within a cell. Noise added to the velocity field causes diffusion between cells. Moments of the displacement were calculated as a function of time while varying the frequency and magnitude of noise in order to magnify the region where sub-diffusion is observed. Frequency of the additive noise extended the time frame in which sub-diffusion was observed and appears to extend the time frame non-linearly. Moments of the displacement show that the diffusive exponent q(s) is the same for all higher moments which indicates scale invariance, or q(s) = constant. This property is characteristic of both anomalous and normal diffusion. The exponent observed $q(s) \sim 0.4$, was larger than the typical exponent of sub-diffusive systems $q(s) \sim 1/3$. The reason for this is undetermined but may indicate an influence of normal diffusion within the system and future investigation is planned.

Composition of Stainless Steel Slurries for Enhanced Structural Support of the TuffCell. *LAURA JANE ELGASS (College of DuPage, Glen Ellyn, IL 60517) J. DAVID CARTER (Argonne National Laboratory, Argonne, IL 60439).* The "TuffCell" is a bipolar plate-supported solid oxide fuel cell that produces electrical power by the galvanic combination of oxygen with hydrogen or other fuel. The SOFC anode support must be both conducting and porous. Porosity is required to ensure that hydrogen gas can flow through the anode support. SOFC anode supports have traditionally been composed of nickel, but the use of stainless steel as a support while also using a thinner anode will provide increased structural integrity. The process for building the support layer starts with making a stainless steel slurry. The slurry composition includes stainless steel powder, binder, plasticizer, solvent, and in some cases pore former. The slurry is allowed to mix thoroughly and is then made into a tape cast using a doctor blade. The tape cast is dried and then placed into the dilatometer for twenty hours where it is exposed to air, nitrogen, and hydrogen to sinter. The weight percent of each slurry component must be such that the slurry meets certain criteria when cast and sintered. In casting, these criteria include an even cast (i.e., the stainless steel cannot separate from the other components during the cast), a strong and flexible dried cast, and a slightly grainy texture. In sintering, the stainless steel layer must not shrink more than the other layers of the cell and must also be porous, with pores approximately 20 microns in diameter. An even cast is the result of optimal slurry viscosity for the given components. Modification of flexibility and strength is accomplished by varying the binder to plasticizer ratio. Porosity can be achieved with a large stainless steel powder particle size and no pore former, or with smaller particles plus pore former (this method warrants varying the volume ratios of stainless steel and pore former to find the optimal porosity). In addition to finding the optimal weight percents of each of the slurry components, it is necessary to determine which plasticizer/binder/solvent trio best casts, sinters, and interacts with the other components of the cell. When xylene/butanol is used for a solvent, compositions with a combination of large stainless steel mesh size and smaller stainless steel mesh size in conjunction with 12% solvent and a plasticizer to binder ratio of 1:5 or 1:7 have proved most successful.

Controlled Assembly of Protein-Mediated Lipid Multi-Bilayers. *CONSTANCE ROCO (University of Virginia, Charlottesville, VA 22904) GABRIEL MONTAÑO (Los Alamos National Laboratory, Los Alamos, NM 87545).* Protein-mediated multilamellar lipid assemblies were created using biotin-streptavadin conjugation. We are interested in using these assemblies as a platform for investigating membranes and membrane-protein properties, as well as towards understanding the relationship between structure and function in biological multilamellar assemblies, such as the neuron insulating myelin sheath. Successive lipid bilayers, containing a fraction of biotinylated lipids, are held together using an intermediate layer of streptavadin. Control over lipid bilayer assembly was determined using atomic force microscopy and spectroscopic ellipsometry. Lateral fluidity of individual layers was characterized by fluorescence recovery after photobleaching (FRAP). Three successive bilayers, with each successive bilayer exhibiting fluidity, have been created. We are currently determining effects of protein concentration and numbers of bilayers on fluidity by comparing rates of diffusion under the various conditions. There are many other properties, such as the substrate and lipid composition, that can affect membrane interactions that can be altered and studied in future work. The investigation of these biomimetic assemblies illustrates how guided molecular self-assembling at the nanometer length scale can improve our understanding of complex biological systems.

Crystallographic Descriptors of a Metal Surface Along a Fracture Line. *RYAN GLAMM (Ohio State University, Columbus, OH 43210) BARBARA K. LOGRASSO (Ames Laboratory, Ames, IA 50011).* This work investigated the feasibility of using electron back scattered diffraction (EBSD) to associate, or differentiate, metal fracture fragments. The objective of this work was to determine an empirical basis for the hypothesis that a minimum sequence of grains can be used to identify a metal fracture line beyond a reasonable doubt. Crystallographic misorientations between individual grains were determined using EBSD along several lines (point-to-origin vectors) of metal crystals within the microstructure of a 304 stainless steel. From a given starting crystal, a grid of vectors was used to do relative referencing comparison of the grain orientation profiles along each vector. A radial grid was used with 5 spacing between vectors at a radius of 11.5 times the average grain diameter. Misorientation angle between grains was calculated by averaging the misorientation angles within a single grain and referencing this average misorientation angle back to the origin grain. The average vector matched 2.6±2 grains with adjacent vectors out of 16.9±7 grains characterized per vector. In point by point matching, vectors placed 5 apart had 83±11% of data points match in the first 2.5 grains away from the origin, with that falling to 36±10% in the last 2.5 grains characterized in the vector. The extent of point to point matching confirms that this method can properly identify when similar or dissimilar profiles are being compared. This leads to the conclusion that a relatively low number of grains need to be analyzed to uniquely characterize a fracture line by relative crystallographic orientations. It also opens the possibility to a more extensive statistical review of concepts and data.

Design, Fabrication and Measurement of Nb/Si Multilayers and Niobium Transmission Filters. *SUNEIDY LEMOS FIGUEREO (University of Puerto Rico, Rio Piedras, Rio Piedras, PR 00931) ERIK GULLIKSON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* The extreme ultraviolet (EUV) region of the electromagnetic spectrum is being used in multilayer optical systems to design technology projected for use in the fabrication of nano-electronics. Multilayer optical systems with high reflectivity have been produced in the soft x-ray and EUV regions of the spectrum. Due to the limited understanding of the Nb/Si optical systems, our research group fabricated and measured Nb/Si multilayers and Nb transmission filters for the soft x-ray and EUV regions. Multilayer optical systems are used in applications ranging from EUV lithography to synchrotron radiation. The films were deposited using dc magnetron sputtering in the Center for X-Ray Optics at the Lawrence Berkeley National Laboratory. Reflectivity and transmission measurements were performed at the Advanced Light Source beamline 6.3.2. The Nb/Si multilayer mirrors fabricated have a reflectivity of approximately 65% in the extreme ultraviolet region, which makes these systems practical for applications where a high reflectivity is required, such as Astronomy and instrumentation development. Transmission measurements of up to 90% were observed in the soft x-ray and EUV regions as well. Future work in the research group includes the design and fabrication of an Nb/Si multilayer with a B4C interface. The Nb/B4C/Si optical systems are expected to have a higher reflectivity than Nb/Si systems.

Detection of Botulinum Toxin with an Automated Fluidics System Using Quantum Dots as the Fluorophore. *ABBY TYLER (Utah State University, Logan, UT 84321) MARVIN WARNER (Pacific Northwest National Laboratory, Richland, WA 99352).* New technologies able to detect biotoxins are in demand as the threat of bioterrorism grows. Effective detection systems have a high sensitivity, allow rapid detection and be automated and accurate. Automated fluidics systems are being developed at PNNL to fulfill all these requirements. The fluidics system performs a sandwich immunoassay that ultilizes high affinity antibodies to detect botulinum toxin. A column of beads, which are conjugated to an antibody specific for a single epitope on the botulinum neurotoxin, are packed above a rotating rod. Next, a liquid sample containing the toxin analyte is perfused over the column. As the sample passes over the column toxin molecules bind to the antibodies on the beads. Then, a dye-labeled antibody that is specific for a second epitope on the toxin is perfused over the column to facilitate binding to the toxin immobilized on the column. Unbound dye is flushed off the column with buffer. Finally, the column is exposed to light to excite the dye and signal the absence or presence of the target toxin. A photo multiplier tube is used to measure the fluorescence of the dye particles left in the column. Many fluorescent dyes are available, and in a series of parallel experiments we have been investigating the use of semicondutor quantum dots as the fluorophore in this detection system. Quantum dots, or semiconductor nanocrystals, are a fluorphore that is becoming widely used in bioimaging though their use in biodetection is relatively new. Some of the advantages that quantum dots have over molecular dyes are that they have a broad excitation spectrum and a narrow emission spectra that is highly red-shifted compared to the excitation wavelength. Further, the wavelength at which they emit can be controlled by the size of the quantum dot. Detection of botulinum toxin using quantum dots in an automated fluidics system was the goal of this research, and is currently under development. Future work will involve improving the overall performance of the system by investigating characteristics such as the non-specific binding of the quantum dots to the column as well as the stability of the antibody coupled materials.

Determining Valence Band Maxima for Photovoltaics Using Ultraviolet Photoelectron Spectroscopy. *SAKA OKYERE-ASIEDU (University of Delaware, Newark, DE 19050) DR. STEVEN HULBERT (Brookhaven National Laboratory, Upton, NY 11973).* Photovoltaic solar cells (PVs) consist of semiconducting materials, which directly convert sunlight into electricity. In order to make high efficiency solar cells there is the need to maximize the transport of charge carriers—thus experiments should reveal energy levels of electrons in the device. Ultraviolet Photoelectron Spectroscopy (UPS) allows for probing these energy levels. In UPS, vacuum UV (10-45 eV) radiation is used to examine valence levels by exciting electrons from those levels. The valence band is defined as the highest electron energies where electrons are normally present and determines the conductivity of the semiconductor. For the experimentation we set three principal goals. The first was to understand the operation of the U4A beamline on which the experiments were run. Since the objective was to study bulk not surface phenomena, it is necessary to understand how to minimize the effects of surface treatment on the measurement. The second goal was then to determine the effect of HF surface treatment on valence bands. Under this goal we needed to identify features in a valence band spectra belonging to the Si substrate, as well as H, O and defects in the Si film. Also, the cross-section for electron excitation and the electron path lengths are incident photon energy dependent. The third goal was to determine the valence band maximum (VBM) for a series of candidate materials for solar cells. This series includes amorphous (a) and crystalline (c) Si, with n-type (n), p-type (p), or intrinsic (i) doping. The series of i-a-Si, n-a-Si, and p-a-Si was analyzed with varying energy photon 30eV – 120eV. For experimental controls, we started with samples of n-c-Si and p-c-Si with expected EF – EV = 0.87eV and 0.225eV. We then compared a-Si films of different p- and n-doping as well as standard i-layer. Future experiments seek to maximize the efficiency of solar cells by adjusting the valence bands using various deposition techniques and doping.

Does an Indentation Size Effect Exist in Nickel Titanium Shape Memory Alloy? *ERIN DONOHUE (Brown University, Providence, RI 02912) EASO P. GEORGE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* Hardness is usually measured by indentation and is considered to be an intrinsic property of a material. Recently, however, an indentation size effect (ISE) has been observed, which is manifested as an increase in a material's hardness with a decrease in the volume of material probed. This phenomenon has previously been studied in a variety of materials and is due to the creation of geometrically necessary dislocations (GND) and work hardening. In this new work, shape memory alloys (SMA) are examined to determine if they demonstrate an ISE. After elastic deformation, instead of going directly into the plastic regime, deformation in a SMA occurs by the reorientation of the variants of the martensite phase. As a result, when the SMA is heated above its martensite-to-austenite transformation temperature, the material returns to its original shape. Nickel titanium (NiTi), a common SMA, is the material chosen for this study. Using an Instron machine, a uniaxial compression test is performed to determine the stress-strain behavior of a bulk sample of NiTi. Another NiTi sample is tested with spherical indenters in the Nano Indenter XP. By making indents at a variety of maximum depths for each of the five indenters of different radii, it is possible to characterize the size dependence of hardness in NiTi. Fused silica, a material whose elastic properties are well known, is used to calibrate the size of each indenter. The indents are also imaged and measured by the MicroXAM Interferometric Surface Profiler. Finally, the sample is placed in hot water to see which indents are able to recover. There is a clear trend of increasing hardness with decreasing radii of the indenters, i.e., an indentation size effect. However, the hardness values obtained with the two smallest spheres were similar, indicating that the size effect breaks down at small length scales. The hardness values obtained with the two largest spheres agree with the hardness deduced from uniaxial compression, indicating that they correspond to the macroscopic hardness of the material. Indent sizes measured with the Nano Indenter and the Profiler correlate well and there is no time-dependent shape recovery. When placed in hot water, all of the indents experience some degree of recovery, with some of the smaller indents disappearing completely. These results indicate that the observed ISE cannot primarily be due to a dislocation mechanism.

Effects of Annealing on DC Sputtered Gold Catalyst for Growth of Pinning-Effective Nanostructures in YBCO Film. *JONATHAN HEBERT (University of South Alabama, Mobile, AL 36688) DAVID CHRISTEN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* As high temperature superconductors move more from the laboratory to industry, it is critical to improve the current carrying capacity. One way to do this is to introduce controllable flux pinning sites, which prevent the dissipative motion of superconducting vortices. A method for this of current interest at ORNL is to embed an ordered array of nanorods within a superconducting film. In order to be effective, this method should produce pinning sites with appropriate sizes in densities comparable to important flux densities, which for most applications is on the order of one tesla. Also, the nanorod material must be nonreactive to the superconductor and, in order to be grown perpendicular to the substrate, have a similar crystal structure to the substrate material. Magnesium oxide (MgO) is an ideal material for these nanorods for use with the superconductor yttrium barium copper oxide (YBCO). Another prerequisite for nanorod growth is the presence of a catalyst, from which the nanorods will nucleate. One such catalyst for MgO is gold. Through the method of DC sputtering, thin films of gold have been fabricated, and by annealing these films, "nanodots" were created. It is known that four main factors affect the size and density of these nanodots: film thickness, substrate material, annealing time, and annealing temperature. In this project the effect of different annealing times was studied for a sputtering time of eight seconds, a sufficient time for the growth of a continuous film, and an annealing temperature of 900°C, the processing temperature of MgO nanorods. Interestingly, the as-deposited film appears to consist of layers of nanoparticles, each around 100 nm in size, implying that the gold is deposited as fairly uniformly sized particles instead of atomically. Analysis of the films and nanodots is carried out using atomic force microscopy and scanning electron microscopy. The results show that an annealing time on the order of tens of minutes is needed for nanostructures to agglomerate from continuous film. In addition, the smallest particles were obtained with an annealing time of 60 minutes, while annealing for 30 minutes produced the most uniformly sized particles.

Electrochemical Characteristics of Secondary Lithium Metal Batteries Containing (x)LiNi0.5Mn0.5O2•(1-x)LiNi0.5Mn1.5O4 as the Active Material in the Cathode. *JACOB HENDRICKS-HOLTZ (Fayetteville State University, Fayetteville, NC 28301) CHRISTOPHER JOHNSON (Argonne National Laboratory, Argonne, IL 60439).* As technology progresses, a search for improved batteries that have higher energy content is needed to implement Li-ion chemistry in hybrid electric vehicles. The (x)$LiNi_{0.5}Mn_{0.5}O_2$ (layered)•(1-x)$LiNi_{0.5}Mn_{1.5}O_4$(spinel) (0 <= x <= 1) composite-structure materials were synthesized and evaluated as cathodes in lithium metal secondary cells. Various lithium metal oxides were synthesized and optimized for phase purity and structure. Electrochemical characteristics are being studied such as current rate, cycle life, stability, capacity, and safety in "coin cells". The synthesis method used was precipitation of the metal hydroxide salts in basic solution, followed by heating the solid with Li_2CO_3 to 900°C in air. For the battery testing the anode was lithium metal, and the electrolyte was a 1.2M of LiPF6 in ethylene carbonate (EC) and ethyl methyl carbonate (EMC) in a ratio of 3:7 respectively as the solvent. Ten charge/discharge cycles were used, with a fully-charged voltage of 4.8V and a fully discharged voltage of 2.8V. The current drawn was 0.16mA with and has a current density of 0.10 mA/cm^2. We used X-Ray Diffraction (XRD) of each metal oxide, (x) $LiNi_{0.5}Mn_{0.5}O_2$ (layered) • (1-x) $LiNi_{0.5}Mn_{1.5}O_4$ (spinel) (0 <= x <= 1), indicated that composites were formed. The composites have broad peaks showing crystal strain in their structure

Electrodeposition of Cobalt and Cobalt-Vanadium Alloy Films on Copper and Iron Substrates. *BENJAMIN TAYLOR (Tennessee Technological University, Cookeville, TN 38505) MARIAPPAN PARANS PARANTHAMAN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* Cobalt (Co) and its alloys have magnetic and electrical properties that are very attractive for technological applications. Low coercivity, high magnetic permeability and relatively high saturation magnetization and electrical resistivity allow these materials to be used in technical devices such as transformers, thin film inductors, giant magneto-impedance sensors, etc. One of the major advantages of Cobalt-Vanadium (Co-V) alloys is that they can be prepared on different shaped substrates with controlled composition and magnetic properties by electrodeposition methods. This study concentrates on developing successful electrodeposition techniques to grow thin films of Co and Co-V alloys on flat Copper and Iron substrates and transform the techniques to round wires. The controlling parameters for electrodeposition of Co and Co-V alloys on Copper and Iron substrates were investigated; these are temperature, pH, current density, electrolyte composition, and time. The compositional, magnetic, electrical, and structural properties of the electrodeposited films were studied. The electroplated samples were characterized using x-ray diffraction (XRD), x-ray fluorescence, scanning electron microscopy (SEM), optical microscopy, atomic force microscopy, and energy dispersive x-ray diffraction. XRD analysis shows that electrodeposited Co forms hexagonal close packed (h.c.p.) and face centered cubic (f.c.c.) structures under the various deposition conditions used in this study. The addition of vanadium (V) and a divided electrolytic cell with very negative current densities forms slightly textured Co films in the (110) and (100) orientations. The division of the cell increases the current efficiency in solutions containing V. Co film thickness is found to have linear relationships with both current density and time. SEM images show dense, uniform Co films without cracks or porosity. Grain size variation is observed with changes in current density and time. More negative current density causes the electrodeposited Co to be deposited f.c.c., which is more magnetically reversible than the h.c.p. structured Co. The coercive field is also significantly less in the f.c.c. electrodeposited cobalt than in the h.c.p. The electrical and magnetic performances of the electrodeposited wires will be compared with commercially available Copper and Iron wires. Research efforts are underway to optimize the growth of Co film alloyed with 2–3 atomic % V.

Examination of Dislocations in Lattice Mismatched GaInAs/GaAs for III-V Photovoltaics. *ALEJANDRO LEVANDER (Pennsylvania State University, State College, PA 16802) JOHN GEISZ (National Renewable Energy Laboratory, Golden, CO 89401).* Dislocations act as sites for nonradiative electron/hole pair recombination, which reduces the efficiency of photovoltaics. Lattice-matched materials can be grown on top of one another without forming a high density of dislocations. However, when the growth of lattice-mismatched (LMM) materials is attempted, many dislocations result from the relaxation of strain in the crystal structure. In an attempt to reduce the number of dislocations that propagate into a solar device when using LMM materials, a compositionally step-graded buffer is placed between the two LMM materials. In order to confine the dislocations in buffer layer, and therefore increase material quality and device efficiency, the growth temperature and thickness of the buffer layer were varied. A GaInP compositionally graded buffer and GaInAs p-n junction were grown on a GaAs substrate in a metal-organic chemical vapor deposition system. A multi-beam optical stress sensor (MOSS) and X-ray diffraction (XRD) were used to characterize the strain in the epilayers. Electrical and optoelectronic properties were measured using a probe station and multimeter setup, solar simulator, and a quantum efficiency instrument. It was determined that device functionality was highly dependent on the growth temperature of the graded buffer. As growth temperature increased, so did the dislocation density in the device despite an increase in the dislocation velocity, which should have increased the dislocation annihilation rate and the diffusion of dislocations to the edge of the crystal. The thickness of the graded buffer also affected device efficiency with thinner samples performing poorly. The thinner graded buffer layers had high internal resistances from reduced carrier concentrations. The empirically derived recipe developed at the National Renewable Energy Laboratory (NREL) produced the highest quality cells. Future work will concentrate on further determining the scientific theory explaining dislocation propagation in LMM buffer layers, possibly by examining the effect of dopant type.

Influence of Charge State and Crystal Structure on Properties of Transparent Conducting Oxide Spinel. *ADRIANA TEODORO-DIER (Lawrence University, Appleton, WI 54912) GREG EXARHOS (Pacific Northwest National Laboratory, Richland, WA 99352).* Solution and vacuum based deposition approaches have been used to prepare thin transition metal oxide films that are electrically conductive. To achieve high conductivity in these materials, processing methods that drive polaron formation in the oxide have been explored. Research reported here is focused on optimizing the transparency and conductivity of $NiCo_2O_4$ and the new polaron conductor $CuMn_2O_4$ by manipulating film deposition parameters. This has been achieved by changing the resident metal cation charge states. Pulsed Laser Deposition (PLD) from a $NiCo_2O_4$ target with high substrate temperature and high oxygen partial pressure followed by post-deposition annealing produced spinel films with resistivities as low as 4.0 x 10-1 Ω cm. In the $CuMn_2O_4$ system, infrared transparent films were deposited from alcoholic or aqueous solutions using spin deposition and PLD. Films deposited from aqueous solutions displayed resistivities of 2.69 Ω cm while those obtained from alcohol solutions were insulating. Although the insulating films became conductive when heated in air, the optimum cation oxidation states to promote conductivity in the films derived from alcohol solutions have not been realized. PLD films of $CuMn_2O_4$ created under conditions similar to those used to deposit $NiCo_2O_4$ films displayed resistivities around 0.5 Ω cm. XRD, XPS, Hall measurements, Raman and transmission spectra were used to further characterize resident properties. Ongoing work involves optimization and refinement of deposition conditions for the $CuMn_2O_4$ PLD films in order to achieve the appropriate mixture of cation oxidation states associated with optimum conductivity.

***Multilayer Mirrors for Extreme Ultraviolet Lithography.** *JONNY RICE (Norfolk State University, Norfolk, VA 23504) DAVID ATTWOOD (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* Extreme Ultraviolet (EUV) lithography promises to be an efficient way to manufacture faster and more powerful microchips. Using light of wavelength 13–14 nm instead of the currently used range of ~200 nm results in the ability to produce smaller feature sizes for the silicon network that makes up the microchip. However, the normal lithography optics cannot be used with this range of light because the scattering of light at this wavelength reduces the rate of success of the process. The answer is multilayer mirrors, mirrors coated with alternating layers of optical materials, since the internal reflections between the individual layers and off-phase refractions within them cause interference that reduces the scatter. The most efficient multilayer optics reflect at ~70%, which means a multilayer mirror must have a high reflectance and be durable enough to withstand the intense energy required for the process, since the initial energy wave will be reduced by 60–70% at each interaction with one of several multilayer optics within the system. Current testing for EUV lithography involves measuring peak reflectance and uniformity of reflectance of mirror samples as well as reductions in reflectance caused by prolonged exposure to radiation. Future research will involve testing new combinations of materials for multilayers as well as testing coating layers designed to lengthen the lifespan of the multilayer optics.

Multiple Differential Aperture X-Ray Microscopy. *OMBREYAN BROADWATER, VIRGIL GREENE (South Carolina State University, Orangeburg, SC 29117) DR. GENE ICE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* A truly non-destructive tool (X-ray microbeam) for three-dimensional (3-D) characterization of mesoscopic and nanoscopic material structures has been developed and is in use. A major breakthrough towards the study of crystal structure distribution in 3-D is the development of Differential Aperture X-Ray Microscopy (DAXM). It provides a way to decode the location of scattering from sites along the incident x-ray microbeam. A single wire DAXM is currently in use. This method has one major drawback; it requires a huge increase in data collection time. In this project, a multiple wire DAXM has been designed and constructed to accelerate 3-D measurements of crystal structure. The design considers beam penetration-depth into the sample, angle of sample surface with respect to beam direction, spacing between the sample surface and the wires, wire size, and wire spacing. An appropriate holder that allows all reflected rays to be detected by the X-ray area detector without interference was also designed and constructed. For a 50-µm diameter size wire, theoretical and computer program data show that data collection time is accelerated by at least a factor of 2.5 compared to a single wire for a 1-µm resolution. Also, a 30 degree angle between sample surface and beam direction resulted in fewer steps and lower minimum wire spacing compared to the 45 degree angle that is currently used. A similar effect is observed as the wires move closer to the sample surface. Multiple-wire Differential Aperture X-ray Microscopy not only accelerates data collection time, but also allows studies of dynamic processes in which short data collection time enables real time resolution. It provides better signal-to-noise-ratio conditions and less sensitivity to instabilities compared to a single wire. This system was tested on the 3D X-ray crystal microscope (station 34-ID-E) at the Argonne National laboratory's Advanced Photon Source and it worked as designed. Detailed analysis and development of software to decode the diffraction information is underway. This result further illustrates the potential for accelerated data collection with multiple differential apertures.

Nitride Membranes: Surface Debris Prevention and Strength Testing. *PATRICK BENNETT (University of California–Berkeley, Berkeley, CA 94720) ERIK ANDERSON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* Fresnel Zone plate lenses are used to focus soft x-rays through a series of alternating zones of opaque and transparent material. Nitride membranes act as a support upon which zone plates are manufactured. The membranes are created by coating a silicon wafer with nitride and then etching away the silicon with potassium hydroxide (KOH) to form a window. Since window strength is an important factor in throughput, it would be desirable to identify and optimize production factors that affect strength. To perform analysis of window strength, an apparatus was designed and constructed that would increase pressure on nitride membranes until breakage, allowing for comparative analysis between different production steps. During testing, it was found that the windows being produced were contaminated with debris. In order to reduce contamination, sources were identified using a process of elimination. By replacing contaminating production steps, surface debris was greatly reduced. Furthermore, debris was eliminated completely using a solution of hydrogen peroxide and sulfuric acid. This is not an ideal solution, however, as it is hazardous and its effects on window strength are unknown. Preliminary results from pressure testing indicate that strength of membranes is dependant on mount orientation. While these results were unexpected, more testing needs to be done to determine the nature of this relationship. Most likely, window strength will be related to both the absolute window size as well as the relative size of window to surrounding silicon support frame.

Non-Destructive Measurement of Residual Stresses in Finished Carburized Gears Using X-ray Diffraction. *BRYAN BOGGS, JEFFREY BUNN (University of Tennessee at Martin, Martin, TN 38238) DR. CAMDEN HUBBARD (Oak Ridge National Laboratory, Oak*

Ridge, TN 37831). Carburization is a common method for improving fatigue strength and wear resistance of gears found in transportation systems. Compressive residual stresses develop as a result of phase transformations from post carburization heat treatments, which improve fatigue strength. Conversely, these phase transformations cause surface distortions to develop in the gear geometry and a loss of surface finish. A finishing process such as grinding or skiving is implemented in order to remove these distortions and improve the finish. This research seeks to quantify the change in residual stress in a carburized gear as it progresses through the finishing process. X-ray diffraction was used to characterize both a finished and unfinished carburized gear to map the residual stresses across and along the face width of a gear tooth. At ten radial positions along the gear tooth, the compressive stresses were measured across the width of the tooth. The unfinished gear showed little variation of residual stresses while the finished gear showed a significantly larger variation of residual stresses. In the unfinished gear the average of the stresses varied slightly and had an average value of 150 ksi compression. However, the finished gear yielded an average compressive residual stress at each radial position that varied linearly from 70 ksi to 130 ksi and then back to 70 ksi. This significant variation is presumed to be a result of the amount of material removed during grinding. Additional tests are planned to determine whether the trends observed from these tests are repeatable for other gear samples. Metrology studies are also in progress to determine the amount of material removed by grinding, with the intent to correlate this loss to the change in residual stress. This research is part of a larger research project in which neutron diffraction will be used to penetrate deeper into the specimen and to compliment the near surface x-ray stress data.

Preparation and Characterization of Self-Assembled Molecular Films. *KYAL WRIGHT (Norfolk State University, Norfolk, VA 23504) MIQUEL SALMERON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* Industrial laboratories and semiconductor manufacturing companies have implemented an initiative to investigate the structure-property relationships, specifically the electrical and mechanical property relationships, of island structures (islands) of organic ultra thin films. Before these properties can be studied, reproducible methods of island formation must be developed to promote controlled structure-property studies. This project will study island formations from alkanethiol self-assembled monolayers (SAM) and conduct preliminary mechanical property tests. There are many parameters that affect the formation of SAM islands. Some of these parameters include the surfactant concentration in solution, the solution temperature, the substrate cleanliness, the substrate's grain sizes and the duration of deposition. This project used Atomic Force Microscopy (AFM) to investigate the relationships between solution concentrations, substrate deposition times, and substrate grain sizes for the control of SAM island domains. To test the effects of deposition time and material concentration on the formation of the SAM islands on gold substrates, alkanethiol molecules in ethanol solution were used in 2 μM, 5μM, 10μM and 20μM concentrations. Experiments dependent on deposition time used time periods ranging from 30 seconds to 6 minutes. Preliminary tests on the effects of flame annealed gold substrates resulted in the use of substrates annealed for 45 passes at one pass per hertz for the tests involving solution concentration and deposition time. The results of the preliminary substrate investigation and structural investigations support that SAM island domains larger than 100nm can be formed on annealed gold substrates when alkanethiol solutions greater than 10μM concentration are deposited on the substrate between 45 seconds and one minute. Results from the mechanical property investigation indicated that the islands formed from 20μM solution at a deposition time of 45 seconds are quite robust when a maximum load corresponding to 8 volts from the AFM system was applied to a 150nm region. While the results from all the investigations support the theory that the first phase of SAM island formation can be controlled, further investigations and trials for each experiment are still needed to confirm this claim.

Processing and Analysis of YBCO Film Spectroscopy Data Using the GRAMS Series of Computer Software. *MICHAEL DUITSMAN (University of Evansville, Evansville, IN 47722) VICTOR MARONI (Argonne National Laboratory, Argonne, IL 60439)*. The Superconductivity for Electric Systems Program at Argonne is performing detailed characterization studies on $Y_1Ba_2Cu_3O_7$ (YBCO) superconducting films deposited on long-length metal substrate tapes. One of the important tools used in this research is Raman microspectroscopy, which makes it possible to determine phase composition and texture quality of the YBCO films. A large number of Raman spectra are collected in this program and each one has to be processed to remove background effects, so that a pure Raman spectrum extrapolated to a horizontal baseline can be obtained for further analysis. Due to the long period of time required to perform even simple mathematical processes on spectroscopy data, there have been many computer programs created to assist in the performance of these tasks. This report discusses the use of one such series of programs-the GRAMS series. The work focused on processing groups of spectra from step-milled samples by applying the software for baselining, noise smoothing, spectral subtraction, and curve-fitting of such spectra. The results show that the GRAMS series facilitates rapid, simple, reproducible processing of spectral data of the type generated by Raman microspectroscopy. The processing of many sets of spectra from a group of six related samples has shown an interesting correlation between the performance behavior of the superconductor and certain types of defects that Raman can detect.

Production of Micro- and Nanocrystalline Diamond Stripper Foils for the Spallation Neutron Source Using Microwave Plasma Chemical Vapor Deposition. *MARK JENSEN (Brigham Young University, Provo, UT 84602) ROBERT W. SHAW (Oak Ridge National Laboratory, Oak Ridge, TN 37831).* Preliminary testing at Brookhaven National Laboratory predicted that diamond stripper foils will have a longer lifetime in the Spallation Neutron Source (SNS) H- beam (38 mA at 1 GeV) than conventional carbon stripper foils. The design of the SNS requires that foils be supported by a single 12 mm edge and extend 20 mm of freestanding foil. Also, the SNS design estimates the ideal areal density to be 280 μg/cm^2 or ~0.8 μm thick. However, testing at Los Alamos National Laboratory showed that increasing foil thickness should provide increased stripping efficiency. Foils were produced using microwave plasma chemical vapor deposition (MPCVD) onto silicon substrates. Substrates were pretreated by the use of ultrasonication in a diamond-methanol slurry. The slurry consisted of 0.3 g each of 35 μm and 4 and 98–99% H_2 at 50 torr. Nanocrystalline diamond films were grown at 900–1000 W in an atmosphere of 1–2% CH4, 8–9% H_2, and 90% Ar at 130 torr. The foils' substrates were then etched using a standard Nitric-HF-Acetic Acid etching solution. Due to thermal expansion mismatch of diamond and silicon, foils originally scrolled upon etching the silicon. To keep the freestanding foil flat, a photolithography technique was used to pattern ~6 μm deep U-shaped channels in the substrate before pretreatment. The channels terminated on the supported edge. Foils showed inconsistent and low nucleation densities that resulted in pinholes and weak areas. Nucleation density increased and became more uniform by frequent stirring of the diamond slurry during pretreatment. This enhancement of the scratching procedure resulted in smoother surfaces and decreased the likelihood of holes. It is anticipated that the usable lifetime of both micro- and nanocrystalline diamond foils will greatly exceed that of conventional stripper foils. The performance of different foils in the SNS will provide direction into which properties and crystal size are the most important for long lasting foils.

Protection of Aluminum from Saltwater Corrosion by Superhydrophobic Films. *PHILIP BARKHUDAROV (Utrecht University, Utrecht, ND 00000) JAROSLAW MAJEWSKI (Los Alamos National Laboratory, Los Alamos, NM 87545).* The damaging effects of corrosion cost billions of dollars each year in metal replacements and repairs. Unfortunately, corrosion cannot be completely stopped; the natural state of most metals on earth is in oxide form. Fortunately, it is possible to slow the oxidation process or to redirect it, and with ever more advanced technology, especially on the nano-scale, corrosion prevention is becoming more and more effective. This research focused on the corrosion of aluminum in salt-water environments. In dry air, aluminum develops a thin surface oxide layer that prevents further corrosion. However, in the presence of water and salt, this layer is broken and rapid corrosion ensues. In this study, superhydrophobic films were layered onto the metal, repelling water and slowing corrosion. These superhydrophobic films consisted of a highly nano-porous silica framework together with hydrophobic organic ligands. To study the effectiveness of such protective layers, the neutron reflectometry method was used. By taking neutron reflection measurements over time on samples of layered aluminum/superhydrophobic film/salt-water, it was possible to observe and quantify the rate of oxide growth in the aluminum. From the relatively short period of measurement, it was possible to predict corrosive behavior on a longer time scale and to show the effectiveness and feasibility of using superhydrophobic films to protect aluminum in marine environments, i.e., ships, off-shore platforms, aircraft, and coastal regions.

Pulsed Laser Deposition of Precursors for Ex Situ BaF_2 Growth of YBCO Superconducting Film. *ALI MORADMAND (University of South Alabama, Mobile, AL 36688) DAVID CHRISTEN (Oak Ridge*

National Laboratory, Oak Ridge, TN 37831). Various methods exist for the deposition of thin films used in materials research of yttrium barium copper oxide (YBCO) superconductors. One common method is in situ pulsed laser deposition (PLD), in which a target is subjected to a pulsed laser beam and ablated into a plume of particles which deposit reactively on a substrate. Another technique used to make high-quality YBCO film for the application of so-called "coated conductor" technology is the ex situ physical vapor deposition of precursors containing BaF_2 at room temperature—unlike in situ PLD where the deposition takes place at elevated temperatures. The precursors are then converted in a furnace to form superconducting YBCO. The focus of this study is to develop a new ex situ PLD method, in which the substrate is kept at room temperature and the deposition of the fluoride-containing YBCO is done using PLD. By optimizing parameters such as ambient gas species, chamber pressure of background gas, and laser energy, YBCO precursors can be formed with the desired thickness, surface morphology, and ratio of the elements in the precursor. The converted films are analyzed for the crystalline YBCO structure using x-ray diffraction and the surface is imaged using atomic force microscopy and scanning electron microscopy. The samples are then tested for superconductivity in a superconducting quantum interference device. Analysis on various samples deposited under different conditions shows that lower laser energy and introduction of background gas can produce film with more favorable surface structure for conversion. Reduction of laser power by modifying the optics reduces the problem of "splashing", which is a known obstacle in PLD. Under an optical microscope, reduction of laser energy shows a significant decrease in surface irregularity. Magnetometry tests show a critical temperature of 88K for these converted YBCO precursor films and critical current densities of 2.9 mA/cm^2 at 5K. Future goals are to further improve film uniformity and quality to increase these values. Because PLD can also make good multilayering films, the long-term goal is to conduct rare-earth substitution into the precursors. Alternating layers of rare-earth material can be deposited in the precursor, and the substitution of the yttrium in YBCO with other rare earth elements has been known to improve flux pinning and raise the critical temperature of such superconductors. By optimizing the parameters for ex situ PLD of a single layer, the method can be extended to rare-earth substituted multilayered precursors as a versatile method of deposition of precursors for high-quality high temperature superconducting films.

Purification of N@C60. *CHANDA ROGERS (Benedict College, Columbia, SC 29204) DR. JOHN SCHLUETER (Argonne National Laboratory, Argonne, IL 60439).* Currently, research is being conducted to produce and purify the endohedral molecule N@C60, which will act as the basic quantum bit (qubit) for the next generation of computers. With these qubits, quantum computers will become more effective in the areas of large database searches, large number factorization, and quantum mechanical simulation of physical systems. Therefore, there is a need to develop methods to increase the yield and purity of N@C60. The method that was chosen for the purification of N@C60 was high performance liquid chromatography (HPLC). Electron paramagnetic resonance (EPR) was used to confirm the presence of N@C60. In utilizing these two methods together, the sample of N@C60 in C60/toluene was separated with the HPLC instrument, and then each fraction from the fraction collector was concentrated down to about 1mL of solution and placed inside of EPR tubes. Next, an EPR spectrum was recorded, and the fraction that gave an EPR spectrum of the clearly defined triplet characteristic of N@C60 was reinjected into HPLC. This will be continued until a pure sample of N@C60 is identified. It will then enter into the next stage of the research, which includes it being formed into the qubits.

Search for Mechanically-Induced Grain Morphology Changes in Oxygen Free Electrolytic (OFE) Copper. *JENNIFER SANDERS (Westminster College, Fulton, MO 65251) ROBERT KIRBY (Stanford Linear Accelerator Center, Stanford, CA 94025).* The deformation of the microscopic, pure metal grains (0.1 to > 1 millimeter) in the copper cells of accelerator structures decreases the power handling capabilities of the structures. The extent of deformation caused by mechanical fabrication damage is the focus of this study. Scanning electron microscope (SEM) imaging of a bonded test stack of six accelerating cells at magnifications of 30, 100, 1000 were taken before simulated mechanical damage was done. After a 2–3° twist was manually applied to the test stack, the cells were cut apart and SEM imaged separately at the same set magnifications (30, 100, and 1000), to examine any effects of the mechanical stress. Images of the cells after the twist were compared to the images of the stack end (cell 60) before the twist. Despite immense radial damage to the end cell from the process of twisting, SEM imaging showed no change in grain morphology from images taken before the damage: copper grains retained shape and the voids at the grain boundaries stay put. Likewise, the inner cells of the test stack showed similar grain consistency to that of the end cell before the twist was applied. Hence, there is no mechanical deformation observed on grains in the aperture disk, either for radial stress or for rotational stress. Furthermore, the high malleability of copper apparently absorbed stress and strain very well without deforming the grain structure in the surface.

Solid Oxide Fuel Cell Based on Proton Conductor. *KATHRYN FENSKE (University of Illinois at Urbana Champaign, Champaign, IL 61820) DR. U. BALACHANDRAN (Argonne National Laboratory, Argonne, IL 60439).* Thin films of $SrCe_{0.95}Yb_{0.05}O_3$-d (SCYb5) are prepared on porous substrates of $SCYb_5$/NiO by a casting method. Dense, crack-free $SCYb_5$ substrate films with a thickness of approximately 10-30μm are successfully deposited on porous NiO/SCYb5 substrates. Scanning Electron Microscopy (SEM) shows uniform thickness of the films and is bonded to the substrate. The prepared cells were tested to determine their performance as a fuel cell at 800°C.

Solvent-Induced Bandgap Effects in Poly(3-hexylthiophene). *RENEE GREEN (University of Pittsburgh, Pittsburgh, PA 15213) GARRY RUMBLES (National Renewable Energy Laboratory, Golden, CO 89401).* Poly(3-hexylthiophene) is a well-studied semiconducting polymer whose absorbance, and thus, optical bandgap, can be altered via formation of thin films or addition of poor solvent. These methods are known to change the color of the polymer from yellow ("Y-form") to red ("R-form"). The change in absorbance of the two forms of polymer results in the widening of its optical bandgap, but the resulting alteration of the electrical bandgap is poorly understood. Absorbance spectra were taken on dilute solutions of poly(3-hexylthiophene) dissolved in THF as methanol was added to bring about the absorbance transition. The resulting absorbance wavelengths were then converted into electron-volts to determine the polymers' optical bandgaps. Cyclic voltammetry was then performed on the solutions containing varying methanol volume fractions to evaluate the polymers' electrical bandgaps. Y-form polythiophene was found to have an approximate optical bandgap of 2.3eV, while that of the R-form was found to be 1.9eV. The electrical bandgap of only the Y-form of the poly was able to be determined, at approximately 1.8eV. Solvent oxidation interference is suspected to be the cause of poor R-form electrochemical data, thus other solvents will be tested. Furthermore, while it is assumed that both phases of R-form polythiophene are energetically analogous, we aim to eventually demonstrate this concept by comparing the electrical and optical bandgap data of the polymer in solution and in thin-film.

Stainless Steel Support Layer for Solid Oxide Fuel Cells (SOFC). *MATTHEW HAMEDANI (College of DuPage, Glen Ellyn, IL 60137) DAVE CARTER (Argonne National Laboratory, Argonne, IL 60439).* The solid oxide fuel cell (SOFC) is a type of fuel cell that operates at high temperatures and employs ceramics as functional elements of the cell. Each cell is composed of a cathode and an anode separated by a solid impervious electrolyte, which during operation conducts oxygen ions produced by reduction of oxygen from the cathode to the anode where they react with hydrogen gas supplied to the anode. This investigation focuses primarily on developing a reliable cell support using stainless steel 434 (SS 434) instead of a nickel cermet support because it is expected to be more cost effective and structurally and chemically durable in hydrogen/steam atmosphere. Ultimately, the cell support layer should have the combined properties of porosity and high electrical conductivity. Layers were made by tape casting onto a Mylar sheet from a pre-made slurry containing metal particles, solvent, binder, plasticizer, and pore former when needed. The binder holds the cast together and makes it viscous, the plasticizer makes the cast flexible, and the pore former which generates porosity in the metal layer once it is sintered. The composition of the slurry was changed so that the cast from it would exhibit the desirable properties of being flexible, smooth, porous, electrically conductive, and sturdy. We found such slurries to be well dispersed, free from foaming and air bubbles, chemically stable, and rheologically optimal for casting. Shrinkage of casts that exhibited desirable properties was measured using a dilatometer. Results indicate that slurries made using butanol as the solvent and B-79 as the binder gave more flexible and sturdy casts than slurries made with Xylene/Butanol as the solvent and AT 746 as the binder. Successful fabrication of multilayer cells containing an electrolyte, anode layers, and two layers of a metal slurry was achieved. Sintering of these multilayer cells at high temperature under controlled atmosphere yielded products in which the electrolyte layer was impervious and free of cracks, while the stainless steel layer displayed the high porosity. Further work will optimize slurry composition and tape casting process.

Structural Investigation of Voids and Al Nanoparticles in 20% Al-80% MoO_3 Thermite Pellets. *JOSHUA HAMMONS (Texas Tech University, Lubbock, TX 79409) JAN ILAVSKY (Argonne National Laboratory, Argonne, IL 60439).* Aluminum and molybdenum trioxide thermites have a very high energy density and thus are a very attractive energetic material. Explosion of these thermites is a result of the oxidation of Al by MoO_3 and some O_2. To enhance the contact of Al particles with the MoO_3, a mixture of 80% MoO_3 and 20% Al was compressed into pellets. When the Al and MoO_3 powders were compressed into pellets, burn rates decreased. The purpose of this research is to gain some insight into the structure of the Aluminum particles and or voids that are in the pellet. Scanning electron microscopy was used to examine the surface of the pellets and compared to ultra-small angle x-ray scattering (USAXS) data performed at Argonne National Laboratory (33-ID beamline). Results indicate the possibility that low density samples contain two separate void phases; the two phases consist of one large void population that is separate from much smaller voids that surround the Al nanoparticles. As the density is increased, the Al particles may penetrate these large voids resulting in a random dispersion of the Al particles in a single void phase. To verify these conclusions additional information is needed. BET analysis should provided additional information about the surface to volume ratio of the void space in these samples. Additional USAXS data should also be obtained on samples that range from 30% TMD to 100%TMD.

Superplastic Forming of Structures Fabricated Using Friction Stir Welding and Friction Stir Spot Welding. *CASSANDRA DEGEN (South Dakota School of Mines and Technology, Rapid City, SD 57701) GLENN GRANT (Pacific Northwest National Laboratory, Richland, WA 99352).* Superplastic forming (SPF) is becoming an increasingly popular metal forming process as parts with more complex shapes are needed. SPF exhibits the ability to form complex near-net shapes, reducing both cost and weight. Welded structures can also be superplastically formed, however the welding method used is critical to the success of the later forming operation. Fusion welded aluminum cannot be superplastically formed because the fusion weld metal is not superplastic. Friction stir welding (FSW) is a new joining method in which the metal is not melted and the microstructure remains fine after welding, an essential requirement for later SPF. In this work, the feasibility of fabricating complex structures using FSW and friction stir spot welding (FSSW) prior to SPF was studied. Coupons of FSW and FSSW were made using different parameters. The coupons were tested in tension at the SPF conditions. Multisheet packs were also made using FSW and FSSW. The packs were then superplastically formed in a superplastic forming press. The results of the coupon and multisheet testing were analyzed and compared to the metallurgy of the welds before and after SPF. Nearly all samples showed abnormal grain growth (AGG), a condition detrimental to the superplastic forming of the weld metal, resulting in low deformation of the weld metal as compared to the parent metal. From these results, recommendations are given concerning which FSW and FSSW parameters should be used to give the best superplastic formability. Future work will include optimizing the weld parameters for SPF and performance testing of the multisheet structures.

Synchrotron X-Ray Diffraction Studies of Single Crystals with Varying High Pressure. *DANIEL SCOTT (Eastern Illinois University, Charleston, IL 60193) YU-SHEN CHEN (Argonne National Laboratory, Argonne, IL 60439).* Three single crystals were studied using a synchrotron resource to understand the change in lattice structure with varying high pressures. The crystal compositions of $H_2C_2O_4$•$2H_2O$, Na_4SiO_4, and $C_{49}H_{40}N_3PS$ were determined by their X-ray diffraction patterns while in the synchrotron beam. The cell parameters of each crystal came out as expected and verified previous research [$H_2C_2O_4$•$2H_2O$: a = 6.100(12), b = 3.500(7), c = 11.850(2), ß = 104.0 (3), Na_4SiO_4: a, b, c = 24.875(2), a, ß, γ = 90.00 , $C_{49}H_{40}N_3PS$: a = 14.624(3), b = 27.343(6), c = 9.982(2), ß = 102.31 (3)]. To apply high pressure to the crystals, ruby fluorescence from an Argon laser was used to determine the pressure calibration of a four-screw Diamond Anvil Cell (DAC). The DAC was calibrated to apply 13.610(5) GPa of pressure over a spectrographic shift of 4.851(7) nm. Due to equipment complications with the DAC, the high pressure lattice determination could not be finished in the specified research time. Future extensions of this research will be to observe how the unit cell of each crystal changes when inside the DAC while being exposed to a synchrotron source.

Temperature Measurements of Lage-Area TCOs under Vacuum. *JENNIFER GADDIS (University of Illinois at Urbana Champaign, Urbana, IL 61801) BRENT NELSON (National Renewable Energy Laboratory, Golden, CO 89401).* The National Center for Photovoltaics (NCPV) has developed new standards for deposition and characterization tools in order to facilitate process development and integration. The first tool designed to these specifications is a sputtering tool for transparent conducting oxides. One such specification dictates that all systems must hold 6” x 6” substrates. Concerns were raised internally at the NCPV about temperature uniformity across the substrates and the performance of large-area heaters. In this study, large area heater characteristics were studied using Type-K thermocouples and an Infrared camera; preliminary work on verifying temperature uniformity and creating intentional non-uniformity was also conducted. Both optical and direct contact measurement techniques were used to create a heater calibration curve for Corning 1737F glass substrates. However, the temperature measured optically was significantly higher due to radiation from the back-plate of the substrate holder. Using the thermocouple measurement, the temperature of the glass was found to achieve only about one half of the heater temperature (°C). For combinatorial deposition, the ability to produce both uniform and intentionally non-uniform heating is desired. An infrared camera was used to create temperature maps of glass substrates. The uniformity of the substrates from 100–400°C was verified to within a standard deviation of 2.6% of the substrate temperature. Intentional temperature reduction of 15% over a specified area of the substrate was produced using a Tantalum radiation shield. Future work will focus on creating a standard temperature measurement method for 6” x 6” substrates, exploration of other materials and thicknesses for the substrate platen, and manipulations of temperature for combinatorial deposition.

The Effect of Phthalocyanines on Solution-Processed Organic Photovoltaic Devices. *TALIA GERSHON (Massachusetts Institute of Technology, Cambridge, MA 02139) DR. SEAN SHAHEEN (National Renewable Energy Laboratory, Golden, CO 89401).* Organic photovoltaics (OPVs) are one mode of renewable energy utilization that promises to provide a cleaner energy alternative to fossil fuels. Initial devices called bulk heterojunctions are commonly made using an active layer composed of a blend of a p-conjugated polymer and a fullerene, in our case poly(3-hexylthiophene) (P3HT) or Poly[2-methyl,5-(3*,7** dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM). These devices have optical band gaps approximately equal to 1.9 eV where an optimal device would have a band gap closer to 1.4 eV, thus adding a third component to red-shift absorption should increase the amount of light absorbed as well as improve the efficiencies of these devices. Liquid crystalline zinc-phthalocyanine (Zn LC PC) and liquid crystalline copper phthalocyanine (Cu LC PC) are materials that have peak absorbances around 650 nm, which would enhance absorption in the active layer in this way; because of their liquid crystalline morphologies, these materials may also improve ordering and, thus, improve transport and efficiency in OPV devices. Other non-liquid crystalline materials that have similar optical densities have also been considered, including a Titanyl Phthalocyanine (TiO PC) and a Free Base Phthalocyanine (Free Base PC). Our research explored the effects of adding such materials to the P3HT:PCBM or MDMO-PPV:PCBM active layers in the bulk heterojunction. Though there is some evidence indicating an improvement in absorption and transport with these materials, no increases in cell efficiency have been observed to date.

The Theoretical Calculation of Phase Diagrams and Thermophysical Properties of Potential Nuclear Fuel Alloys. *COREY WESTFALL (Albertson College of Idaho, Caldwell, ID 83605) IRINA GLAGOLENKO (Idaho National Laboratory, Idaho Falls, ID 83415).* With the increase of nuclear power plants, nuclear waste is becoming an increasing environmental concern. By transmuting the Actinides in a burner reactor, the amount of nuclear waste can be decreased significantly. Zirconium based alloys have been considered for use in burner reactors, but due to the rarity and dangers of the Actinides, little, if any, Actinide-Zirconium alloy data exists. To supplement this data, Thermo-Calc®, a thermodynamic modeling software, was used in conjunction with TCNF2®, a nuclear fuel database, to create phase diagrams and property plots for the Actinide-Zirconium binaries, a pseudo-binary for Am-Pu-Zr, and multiple ternaries for U-Pu-Zr. The graphs were then compared to experimental plots to identify errors in TCNF2® and to determine the alloy data needed to correct the database. The melting temperatures were calculated for multiple alloys of interest in burner reactors. Thermo-Calc® was shown to perform very well calculating the melting temperatures and most of the binaries, but TCNF2® was shown to be lacking data for Np-Zr, most Americium alloy data, and ternary data.

Future work includes the characterization of the recommended alloys and that incorporation of this data into TCNF2®.

Ultrasonic Testing of High Attenuation Materials with Pulse Compression Techniques. *LISA DEIBLER (Washington State University, Pullman, WA 99164) BRIAN TUCKER (Pacific Northwest National Laboratory, Richland, WA 99352).* Homeland security and industry widely employ ultrasonic non-destructive evaluation (NDE) because of sound's ability to non-invasively characterize a variety of materials. However, the capabilities of conventional ultrasonic NDE are severely limited in many materials due to high attenuation and scattering of ultrasound. In addition, most ultrasonic techniques require contact with the specimen either by immersion or direct coupling, which can present issues for moisture-sensitive materials and/or materials in a high-speed process line. Recent advances in air-coupled transducers have enabled the efficient transmission of broadband ultrasonic (between 20 kHz and 1.5 MHz) waveforms through air, eliminating the need for specimen contact. Additionally, pulse compression, a technique commonly used in RADAR applications, provides a higher signal-to-noise ratio (SNR) for accurate measurements. Combining air-coupled transducers with pulse compression shows great promise for characterizing ultrasonically difficult materials without the need for specimen contact. Comparison of two pulse compression techniques, cross correlation (XCorr) and swept frequency multiplication (SFM), by computer simulations and experimental testing revealed a more robust and accurate response from XCorr. Using air-coupled transducers and the XCorr pulse compression method, SNRs up to 28.3 dB (increase of 26 times in signal strength) over conventional ultrasound were observed. This method was used to successfully detect a defect in a thick (10mm) carbon fiber laminate without the need for direct specimen contact. Combining advanced signal processing techniques with the capabilities of broadband electrostatic transducers is shown to be a highly promising non-contact method for characterizing difficult materials in air.

X-ray Photoelectron Spectroscopy of GaP(1-x)N(x) Photocorroded as a Result of Hydrogen Production Through Water Electrolysis. *MARIE MAYER (University of Illinois at Urbana Champaign, Urbana-Champaign, IL 61801) ANDERS NILSSON (Stanford Linear Accelerator Center, Stanford, CA 94025).* Photoelectrochemical (PEC) cells produce hydrogen gas through the sunlight driven electrolysis of water. By extracting hydrogen and oxygen from water and storing solar energy in the H-H bond, they offer a promising renewable energy technology. Addition of dilute amounts of nitrogen to III-V semiconductors has been shown to dramatically increase the stability of these materials for hydrogen production. In an effort to learn more about the origin of semiconductor photocorrosion in PEC cells, three samples of p-type GaP1-xNx (x = 0, 0.002, 0.02) were photocorroded and examined by X-ray Photoelectron Spectroscopy (XPS). GaPN samples were observed to be more efficient during the hydrogen production process than the pure GaP samples. Sample surfaces contained gallium oxides in the form of Ga_2O_3 and $Ga(OH)_3$ and phosphorus oxide (P_2O_5), as well as surface oxides from exposure to air. A significant shift in intensity from bulk to surface peaks dramatic nitrogen segregation to the surface during photoelectrochemical hydrogen production. Further investigations, including using a scanning electron microscope to investigate sample topography and inductively coupled plasma mass spectroscopy (ICP-MS) analysis for solution analyses, are under way to determine the mechanism for these changes.

X-ray Reflectivity Characterization of Structural Damage Induced by Xe^+ Bombardment in Thin Film EUV Collector Mirror Optics. *DOUGLAS DETERT (University of Wisconsin–Madison, Madison, WI 53711) JEAN-PAUL ALLAIN (Argonne National Laboratory, Argonne, IL 60439).* Xe^+ ion bombardment produced by extreme ultraviolet (EUV) plasma-based sources degrades the surface and limits the operational lifetime of single layer and multilayer thin film collector optics used in 13.5 nm wavelength EUV lithography. The objectives of this experiment are twofold: to use specular Cu Kα1 (α=1.54 Å) X-ray reflectivity (XRR) analysis to characterize and quantify the structural damage induced by Xe^+ bombardment in multilayer mirrors, and to predict the 13.5 nm wavelength (EUV) reflectivity performance of both single layer and multilayer mirrors using traditional 1.54 Å wavelength XRR. Si/Mo multilayer films were subjected to 1 keV Xe^+ fluences ranging between 10^{16} to 10^{16} Xe^+/cm^{-2} at temperatures of 294 and 473 K. In addition, both EUV and Cu Kα1 wavelength XRR analyses were performed on non-irradiated Ru/Ti single layer films. A systematic comparison of XRR simulations using IMD software and measured XRR data at a wavelength of 1.54 Å reveals that while the simulations provide useful insight into the interaction of thin films and X-rays, the specific scheme used may be inadequate for obtaining accurate structural information about the irradiated mirrors or reflectivity behavior at 13.5 nm. The behavior of single layer mirror reflectivity at Kα1 scales well in IMD simulations to predict the measured EUV reflectivity performance at 13.5 nm. This work is part of an ongoing study that seeks to understand the EUV reflectivity performance of thin film collector mirrors and the combined effects of damage in EUV lithography optics from energetic ion-bombardment, thermal deposition of neutral particles, and off-band radiation produced by Xe^+ and Sn^+ plasma-based light sources.

Medical and Health Sciences

A Noninvasive Method to Assess Left and Right Ventricular Fractional Area Change in Genetically Altered Mice. *MEAGAN GREEN (La Salle University, Philadelphia, PA 19141) HELENE BENVENISTE (Brookhaven National Laboratory, Upton, NY 11973).* The techniques which allow a comprehensive assessment of cardiovascular performance in small animals are still limited. The development of a noninvasive cardiac MRI- based method to facilitate the analysis of both right and left ventricular function in a mouse heart is essential in a cardiac study. The use of animals with genetic modifications, which lacks the ability to produce vasointestinal peptide (VIP), and important cardiovascular regulatory factor. The use of these animals with genetic modifications allows for a more precise assessment of cardiovascular failure development. Changes in myocardial VIP concentration or with alteration of physiological responsiveness of VIP receptors have been links to the development of severe cardiovascular disorders, such as myocardial fibrosis, heart failure, cardiomyopathy and pulmonary hypertension. The goal of this study was to compare the left and right ventricle to see if they are both equally involved in the development of cardiomyopathy in VIP-deficient mice. The cardiac imagine was performed in five anesthetized animals using several different Flash_movie sequences in a 9.4T MicroMRI system. Once the images were obtained Amira Imaging software was utilized to make outlines of the left and right ventricular cavities and areas for each ventricle were obtained during different phase of the cardiac cycle. A transactional view through the midpapillary level was used for analysis. Functional ventricular assessment was performed by calculating the fractional area change (FRAC) during systole. Data showed that there was not a significant difference between the left ventricle (53.87 +/- 13.66%) and the right ventricle (52.90 +/- 15.01%) FRAC. Both sides developed significant hypertrophy of the myocardial wall. In summary, the VIP- deficient mouse, the development of cariomyopathy was shown to similarly affect both the left and right ventricular function. We were able to develop a noninvasive method for advanced characterization of cardiac function in the murine model. This will help to facilitate longitudinal study of the heart disease process. The long term goal of this study is to map the development of heart disease.

An Examination of Perseveration in Cocaine Abusers. *TANYA LUKASIK (Stony Brook University, Stony Brook, NY 11794) RITA GOLDSTEIN, PH.D. & PATRICIA WOICIK, PH.D. (Brookhaven National Laboratory, Upton, NY 11973).* Drug addiction is associated with executive deficits that are typically attributed to dysfunction in prefrontal brain regions (e.g., the ventromedial region of the orbitofrontal cortex and dorsolateral prefrontal cortex). Cocaine-addicted individuals exhibit mild performance deficits on neuropsychological tasks that require set shifting, instead, perseverating on previously rewarded behavior. However, the research reported is inconclusive possibly due to the heterogeneity among cocaine-abusing populations. In the current study, cocaine abusers were compared to healthy control subjects on the Wisconsin Card Sorting Task, (WCST); a classical neuropsychological task that assesses concept formation, cognitive flexibility and set shifting. Cocaine abusers were grouped according to their ability to complete all categories on the WCST (high functioning versus low functioning). Compared to higher functioning cocaine subjects, lower functioning cocaine abusers were associated with more positive urine screens. Lower functioning cocaine subjects also scored lower on indices of general intelligence and traditional indices (total scores) of the WCST as compared to higher functioning cocaine subjects and controls. In contrast, higher functioning cocaine abusers scored similarly to controls on total scores of the WCST, however, an examination of performances at the category level suggests a different pattern of learning, specifically a tendency to perseverate in the first sequence of the task. Results suggest two patterns of executive dysfunction in cocaine abusers; one associated with lower functioning cocaine abusers that is more severe and possibly related to acute withdrawal (recent cocaine use) and another associated with higher functioning cocaine abusers characterized by mild perseverative deficits.