2019 Materials Science Graduate Student Symposium

Abstracts

Session I – Magnetic Materials

Oral presentations

The magnetic spin textures in FeGe thin films

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Currently, systems with stable skyrmion behavior at room temperature require engineered heterostructures for realization, as the Skyrmionic material with the highest Curie Temperature remains FeGe at 278K at bulk [1], and low magnetic moment at room temperature when strained on Si substrates (T_C ~ 275K) [2]. We have synthesized and studied the magnetic properties of strained FeGe thin films of thickness 20 nm, 40 nm, 80 nm and 115 nm, prepared by D.C. magnetron sputtering of Fe and Ge targets on Ge (111) substrate. The magnetic characterization of FeGe thin films showed an enhanced transition temperature of T = 341K. The preliminary results from FMR measurements suggest helical magnetic structure in these thin films. The Lorentz transmission electron microscopy and neutron diffraction measurements are underway to characterize the Skyrmionic and magnetic structure.

[1] N. Nagaosa and Y. Tokura, Topological properties and dynamics of magnetic skyrmions, Nat. Nanotechnol. 8, 899 (2013).

[2] J. C. Gallagher, K. Y. Meng, J. T. Brangham, H. L. Wang, B. D. Esser, D. W. McComb, and F. Y. Yang, Phys. Rev. Lett. 118, 027201 (2017)

Dzyaloshinskii-Moriya Interaction in Ultrathin Films and Multilayer Structure for Domain Wall Skyrmions

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Magnetic Skyrmions are topologically protected spin textures which are promising candidates for spintronic and spin logic devices. They can be realized in bulk systems with broken inversion symmetry or in ultra-thin multilayers with broken symmetry at the interface. Two key parameters in those thin films structures are perpendicular anisotropy and Dzyaloshinskii-Moriya interaction (DMI). Both effects depend strongly on spin-orbit coupling at the interface between the ferromagnetic and non-magnetic layers. Our aim in this project is to understand the microscopic origin of DMI at Pt/Co, and Ir/Co interfaces and its connection to the surface anisotropy in those multilayers. We use first principle based on density functional theory to determine the perpendicular anisotropy and DMI vectors. The result guides experimental efforts to stabilize a new form of magnetic skyrmions, the so called Domain wall Skyrmions.

Acknowledgements

Part of this research is supported by the Defense Advanced Research Project Agency (DARPA) program on Topological Excitation in Electronics (TEE) under grant number D18AP00011 and NSF 1452670. Further, we would also like to acknowledge the support of the University of Alabama High Performance Computing facilities and staff.

Computational Materials Science: Electronic Structure of Nanocrystalline Soft Magnetic Materials

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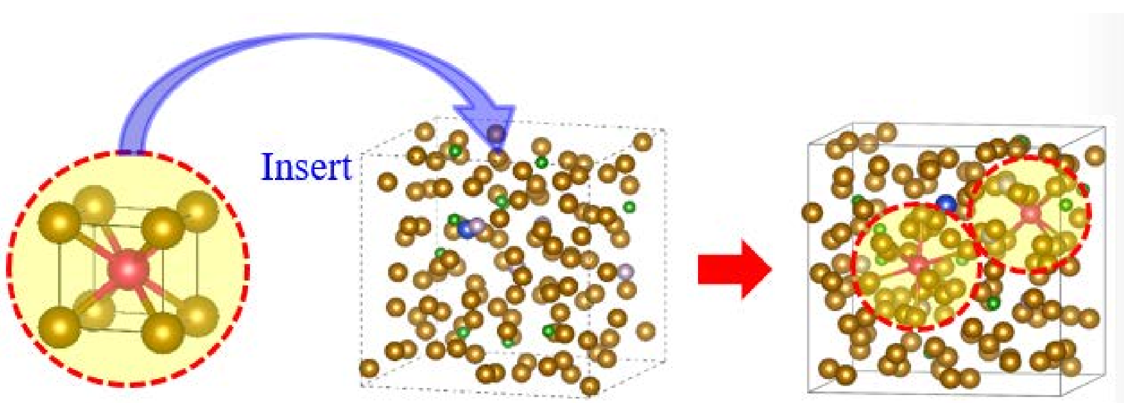
The nanocrystalline soft magnet consists of Fe-based nanocrystallite and amorphous matrix. We have previously developed the calculation methodology for the electronic structure of nanocrystalline Fe-Cu-Si-B soft magnet [AIP Advances **6**, 055915, 2016]. In this methodology, we have calculated the electronic structure of nanocrystallite (Fe_3Si) and amorphous matrix (Fe-B), separately, using first-principles calculations. To include the magnetic interaction between ferromagnetic crystallite and weak ferromagnetic matrix in our new calculation methodology, we have embedded nanocrystallites (Fe-Co) into the amorphous matrix (Fe-B-P-Cu), then calculated the electronic structure of the crystallite embedded soft magnet. First, the *ab initio* molecular dynamics was performed to prepare the amorphous matrix by randomly distributing the atoms in the amorphous matrix. Then, we embedded two crystallites into the amorphous matrix. Figures show crystallite and crystallite embedded nanocrystalline soft magnet. As a result, the total magnetic moments (μ_B) is 249.01 for 2 crystallites. These magnetic moments convert to the magnetic flux density of 1.91 T for 2 crystallites. The new calculation methodology shows the same results as our previous methodology but considers the magnetic interaction between nanocrystallites and the amorphous matrix, therefore, more accuracy. We will introduce the new computational methodology. We will introduce our new computational methodology.



Ferromagnetic Nanocrystallite Amorphous Matrix Nanocrystalline Soft Magnet

Broadband FMR measurements on MnN/CoFeB exchange biased systems

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In exchanged bias systems, the interfacial exchange coupling between a ferromagnetic layer and an antiferromagnetic layer, creates a unidirectional anisotropy in the ferromagnetic layer which manifests in the form of a shift in the hysteresis curve [1]. In this work, we performed broadband ferromagnetic resonance measurements on MnN(30nm)/CoFeB(t_{CoFeB}) bilayer systems with t_{CoFeB} ranging from 5 to 20nm. In the broadband ferromagnetic resonance measurements, the static external magnetic field was applied parallel and antiparallel to the exchanged bias direction. Besides the unidirectional anisotropy we also observe an additional uniaxial anisotropy. In-plane angle dependent measurements were also performed to better understand and quantify both anisotropies. Based on this data we were able to quantify the interfacial exchange coupling $\Delta\sigma = 0.206 \pm 0.003 (emu/cm^2)$ for our samples. Our results also confirm the presence of a unidirectional relaxation mechanism [2,3] along with uniaxial relaxation mechanism in this system. Consequently, the effective Gilbert damping parameter is different for parallel and antiparallel orientations.

References

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2. Mewes, T., et al., *Unidirectional magnetization relaxation in exchange-biased films*. IEEE Magnetics Letters, 2010. **1**: p. 3500204-3500204.
3. Mohammadi, J.B., et al., *Broadband ferromagnetic resonance characterization of anisotropies and relaxation in exchange-biased IrMn/CoFe bilayers*. Physical Review B, 2017. **95**(6): p. 064414.

Thickness Dependence of Magnetization Dynamics of (FeCo)-Si Alloy Thin Films

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$(Fe_{75}Co_{25})_{95}Si_5$ alloy thin films of various thicknesses were deposited on MgO(100) single crystal substrates by magnetron sputtering at 230 °C substrate temperature. The thickness dependence of both quasi-static and dynamic magnetic properties were investigated by vibrating sample magnetometer (VSM), magneto-optical Kerr effect (MOKE) and broadband ferromagnetic resonance (FMR). The X-ray diffraction (XRD) results indicate that all films are of the bcc structure with an in-plane epitaxial alignment of $[100]_{FeCoSi}$ // $[110]_{MgO}$. The exchange constant was determined from the field shift between the uniform precession FMR mode and the first order perpendicular standing spin wave (PSSW) resonance mode in the FMR spectra. The effective damping parameter decreases dramatically with increasing film thickness up to 16 nm due to the decrease of the spin pumping contribution and then remains relatively constant as the film thickness increases. In-plane angle dependent FMR measurements reveal that the in-plane anisotropy of these films is dominated by a four-fold magnetic anisotropy, which increases sharply with increasing film thickness up to 16 nm and then shows a slightly decreasing trend as the film thickness increases. In-plane angular dependence of the FMR linewidth shows a strong two magnon scattering contribution.

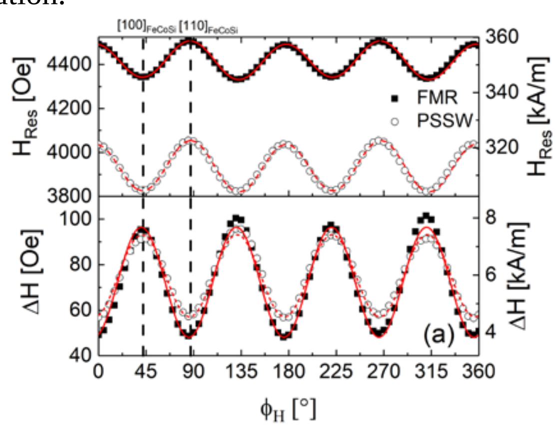

Figure 1. In-plane angular dependence of the resonance field and linewidth for the 82 nm thick $Fe_{69}Co_{26}Si_5$ film at 30 GHz. The solid squares and open circles represent the FMR mode and PSSW mode, respectively. Red lines correspond to fits to the data.

Session II – Advanced Manufacturing Materials

Oral presentations

Finite element failure analysis of addictively manufactured lattice structure

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Abstract

Lattice structures offer high strength and stiffness/mass ratio features which provide freedom in design that is beyond the solid materials capacity, however they have natural tendency to develop localized failures due to large number of thin struts building the structure. Accordingly, collapse of few struts has a great impact on the global strength and stability. Therefore, the objective of this study is to answer this question that where and how failure initiates and propagates through the additively manufactured lattice structures made of Nickel based super alloys. Inconel 718 shows different behavior in tension and compression, therefore the modified volumetric hardening model (VHM) along with damage initiation and propagation criteria are implemented to quantify damage in the lattice structure subjected to quasi-static loading. The results are in a good agreement with experimental results.

A Transient Thermal Model for Predicting Thermal Gradients in Additive Manufacturing Using the Finite Difference Method

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Numerical thermal modeling of metal additive manufacturing (AM) processes is typically very computationally expensive. Being able to simulate the complex physics of melting and solidification requires very fine meshing in both space and time. While state of the art numerical models have been developed that offer great insight into these processes, they require powerful parallel computational capabilities and days/weeks of processing time. A new approach has been developed that simplifies the transient thermal modeling in AM processing and can be run on a typical desktop computer without the use of parallel processing. This transient model predicts the resulting thermal gradients in real time that is faster than the time required to build most parts. The modeling takes advantage of the simplicity of the finite difference method to develop a unique method of node creation. Computational time is reduced by meshing in both space and time along with simplifying assumptions about the process of solidification. This results in a model which predicts temperature gradients that track with those found in experimental measurements. Because its light computational expense, it is envisioned that this method could be developed as a useful tool in industrial applications to optimize print pathing to reduce the thermal gradients and thereby the residual stresses.

Measurement of Residual Strain in High Pressure Die Cast A383 Engine Blocks Using Neutron Diffraction

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Abstract

The residual strains in three high pressure die cast A383 engine blocks are measured by using neutron diffraction in this work. Residual strains and stresses can be generated during high pressure die casting process due to the thermal gradients and may cause premature failure or distortion. Neutron diffraction can be used to measure the residual stress distributions deep inside castings with complicated geometries, as neutrons have much larger penetrating power than X-rays. In the present work, the residual strains (in the axial and hoop directions) along the whole cylinder bridge of high pressure die cast A383 engine blocks in as-cast and heat-treated conditions were measured by neutron diffraction method. The effect of heat treatment on the distribution of residual strains was also investigated. The results suggest that the residual strain in the cylinder bridge is tensile in both the axial and hoop components for both as-cast and heat-treated engine blocks. The residual strain in the hoop direction is larger in magnitude than the residual strain in the axial direction. Heat treatment remarkedly relaxes the residual strain in the axial direction but only slightly relaxes the residual strain in the hoop direction.

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Exploring variability in the microstructural response and mechanical properties of heat treated blown powder Inconel 625

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The blown powder process is a prominent method of additive manufacturing in which metal powders are blown into a laser beam attached to a robotic arm. The laser and robotic arm melt and distribute the powders based on the design of the component being fabricated. The powders then metallurgically bond upon cooling to form a solid structure. The blown powder method is preferred when additively manufacturing larger components, which is especially useful for aerospace applications. After fabrication, various heat treatments are needed to relieve residual stresses that developed during the manufacturing process, as well as to optimize the material's mechanical properties. This study explores the effects of heat treatments held at various temperatures on the microstructure and mechanical properties of Inconel 625, a nickel-based superalloy manufactured using the blown powder AM process. The material was provided by four vendors to address similarities and variabilities in each specimen's response.

Quantifying bimetallic joints formed using direct metal deposition processes for an additive manufactured rocket engine component

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To reduce costs associated with the fabrication of complex rocket engine components, various additive manufacturing (AM) processes are being explored. While processes, such as selected laser melting (SLM) can print monolithic components, other more complex components require a combination of Cu for conductivity and a higher strength-lower density material such as Inconel, for structural stability. The application of direct metal deposition (DMD) processes can be used to print these bimetallic components. This approach greatly reduces the time and hence cost by eliminating multiple processing steps, such as brazing, to fabricate the multi component heritage hardware. Although use of blown powder DMD was recently used to fabricate an RS-25 augmented spark igniter (ASI) that was hot fire tested in July 2017, little is known about the reliability and stability of the resulting interface formed as the metals are directly deposited on one another. This proposed effort would quantify the material properties of the bimetallic interface and evaluate its stability at elevated temperatures. Specimens proposed for this study have been fabricated by 3 different vendors using 2 different DMD processes. By quantifying the bimetallic joint, the overall technical readiness level (TRL) of an additively manufactured component can be increased.

Modeling of a Hyperbaric-Pressure Laser Chemical Vapor Deposition

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Chemical vapor deposition (CVD) is a process that takes a precursor gas, usually a solid material in a volatile form, and deposits that material onto a heated substrate by a chemical reaction occurring due to the heat. Laser chemical vapor deposition (LCVD) is a type of CVD that uses a laser beam to heat a small section of the substrate, thus starting the vapor deposition reaction. This creates a local CVD reaction and allows for specific patterns of the deposited material to be created. This also allows for three-dimensional CVD to take place. If the focal point of the laser is moved away from the substrate, the reaction follows and results in the formation of a fiber composed of the deposited material. The purpose of this study is to model the flow and temperature of a laser chemical vapor deposition reaction by means of a multiphysics software. Varying parameters in the reaction chamber has been shown to affect the quality of the fibers produced. The pressure in the reaction chamber during growth is the specific parameter that will be varied. The results will be analyzed and will give insight as to how this will change the process of LCVD.

Evaluation of the Orthogonal Metal Cutting Process for Characterizing the Microstructural Evolution in Friction Stir Welding

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The friction stir welding (FSW) process in metals results in a microstructure consisting of fine grains in random orientations. Estimates of the hot working conditions during a FSW are in the range of 50 to 100 for the shear strain and 10^3 to 10^6 s^{-1} for the shear strain rate. The process parameters controlling the grain refinement are not well understood and test methods to reproduce the hot working conditions in laboratory experiments are lacking. Understanding this microstructural evolution and its relationship to process parameters during FSW is essential for anchoring predictive models. Currently, the development of process parameters for the FSW process relies upon trial and error. The shear surface that forms around the tool during FSW is similar to the shear plane formed during orthogonal metal cutting. Since the algorithms have been developed for calculating the shear strain and shear strain rate during metal cutting, it is proposed to adapt this test method to screen metal working conditions for producing the desired microstucture in a FSW. Thus, metal cutting is being explored as an experimental test method for linking microstructural evolution to the hot working conditions of temperature, strain, and strain rate.

Volumetric Fatigue Crack Quantification of α-Iron

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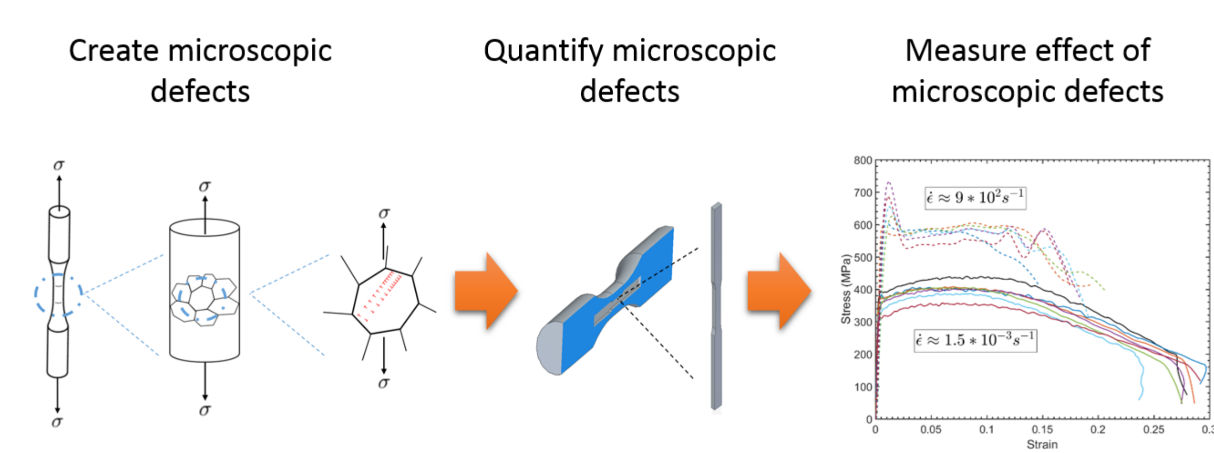
This is the first ever work to quantify the evolution of bulk material defects generated during cyclic elastic loading and the subsequent effects those defects have on quasi-static and dynamic mechanical behavior. Fatigue cracks typically begin at the surface then crack propagation and failure originate from that location. Often overlooked are changes the bulk material may experience as a result of cyclic loading. This type of bulk microscopic evolution is important if parts and components are to be extended past their intended service life to ensure mechanical performance is not degraded and still meets design requirements. In this work fatigue test specimens of pure iron were cycled at 70% of the yield stress to introduce elastic defects throughout the material. Afterwards, wire-cut electrical discharge machining was used to obtain multiple sub-tensile specimens from within the gauge section of the fatigued material. X-ray computed tomography was used to quantify distribution and location of volumetric voids and defects induced at different fatigue life stages of the sub-tensile specimens. Then, tension tests were performed on the sub-tensile specimens at low, $10^{-3}s^{-1}$, and high, $10^{3}s^{-1}$, strain rates to study changes in mechanical properties.



Bulk microscopic defects are accumulated during elastic, load controlled fatigue (left). Volumetric defect evolution in the fatigued material is quantified using X-ray computer tomography (center). Mechanical properties are measured under quasi-static and dynamic loading to correlate changes due to the defect evolution (right).

Transmission Kikuchi Diffraction of the Thermally Grown Oxide on Grain-refined NiAl-Zr

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Grain refinement of high temperature oxidation resistant materials has been shown to expedite oxide phase transformations and improve spallation resistance. However, very little work has been done to investigate the resulting oxide microstructure in detail. The present study correlates the oxidation behavior to the oxide microstructural features of grain-refined overdoped NiAl-0.09Zr and extruded NiAl-0.05Zr (at.%) using secondary electron microscopy (SEM), transmission electron microscopy (TEM), and transmission Kikuchi diffraction (TKD). Grain refinement was achieved by DC magnetron sputter deposition. Figure 1 shows bright field TEM and the TKD band contrast map of the three-layer oxide that was found to grow on sputter deposited NiAl-Zr after 50 h of oxidation. TKD phase identification, not shown here, confirms the presence of monoclinic and tetragonal ZrO_2 within the fine grained middle oxide layer. Formation and growth of this three-layer structure will be discussed with respect to the reactive element effect on oxide scale morphology, growth mechanism, and spallation resistance.

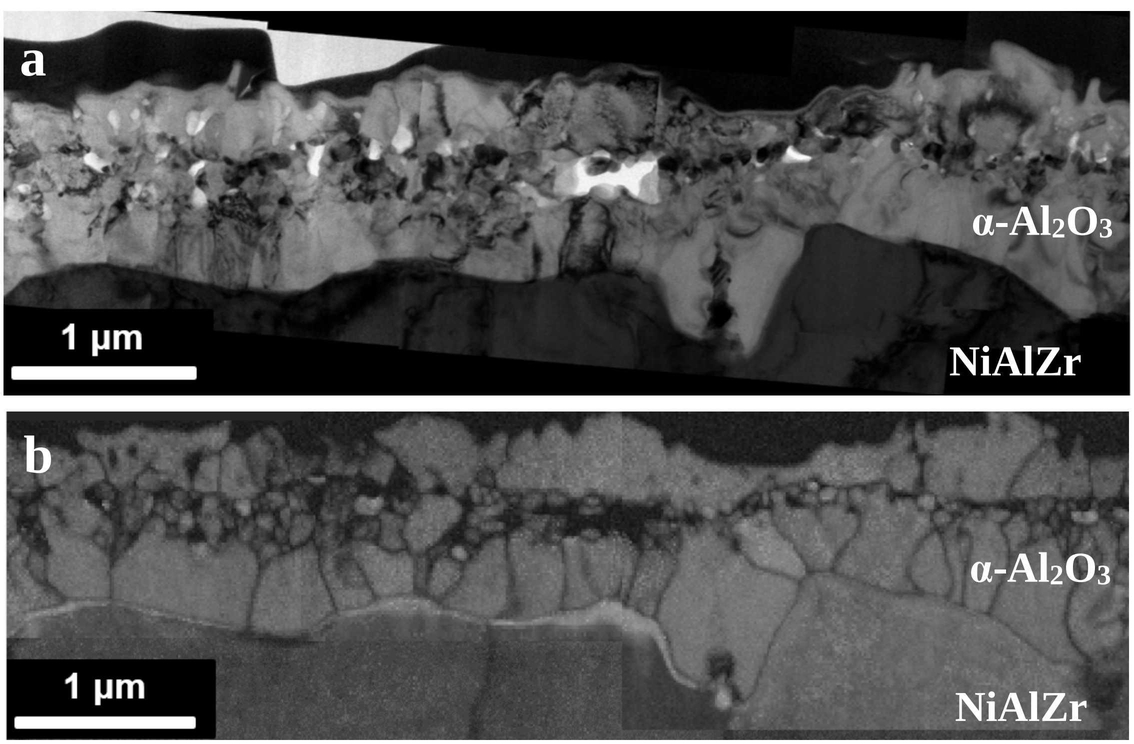

Figure 1: (a) TEM bright field and (b) TKD band contrast map showing the three-layered oxide grown on sputter deposited NiAl-Zr after 50 h of oxidation at 1000°C

Session III – Energy materials

Oral presentations

Design of segmented high-performance thermoelectric generators with cost in consideration

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The state-of-the-art thermoelectric (TE) materials working between 300 K and 1000 K are cautiously selected, including Chalcogenides, SiGe alloy, Skutterudites and Half-Heuslers. The selection principle is an overall reflection of the figure of merit (*ZT*), compatibility factors and power factors of TE materials. These chosen TE materials are divided into four groups for construction of two kinds of segmented p-type TEG legs and two kinds of segmented n-type TEG legs. Built on different combinations of these segmented TE groups, thermoelectric generators (TEGs) have been systematically modelled to find out the best cost-performance ratios and the corresponding efficiencies, output power densities and TEG geometries as well. All the TE material properties input in the simulation are temperature-dependent and the electrical & thermal contact resistances have been taken into account for every TE-TE and TE-electrode interfaces. The results demonstrate that successful segmentation of high-*ZT* TE materials can offer a cost-performance ratio of ~0.86 $ W^{-1}, less than commercially desired cost-effectiveness of 1 $ W^{-1}, while maintaining an efficiency of 17.8% and delivering a power density over 3 Watt cm^{-2}. These results predict the commercial feasibility and competitiveness of segmented TEGs in the same dollar per watt metrics as other renewable energy sources.

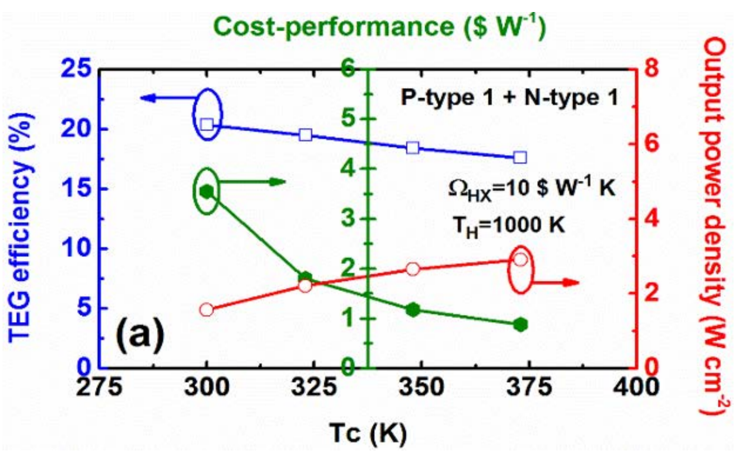

Figure. Cost-performance, TEG efficiency and output power density versus the cold-side temperature of TEG module.

Insight into the Synergism of CeO_2NR Supported M–Co Bimetallic Oxides (M=Fe, Ni, Cu) for CO Oxidation Reaction

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Supported bimetallic catalysts with the rational compositions and structural design have attracted great interest, due to the enhanced catalytic activity, selectivity or stability etc. In this study, 10 wt% Fe-Co, Ni-Co and Cu-Co bimetallic oxides with 1:2 atomic ratios ($FeCo_2O_x$, $NiCo_2O_x$ and $CuCo_2O_x$) and Co-Cu bimetallic oxides with different ratio of 1:2, 1:1 and 2:1 (Cu_2CoO_x, $CuCoO_x$ and $CuCo_2O_x$) were deposited onto the surface of CeO_2 nanorods (CeO_2NR) through a hydrothermal-assisted precipitation-deposition method. The goal of this study aims at understanding the effects of bimetallic synergism, surface structure configuration and support reducibility. The catalysts were mainly characterized by means of XRD, Raman Spectroscopy, XPS, TEM, N_2-BET, H_2-TPR, TPD and O_2-pulse chemisorption. Hydrogen and carbon monoxide were employed as the probe molecule to testify their reducibility and the catalytic performance. 10% Cu_2CoO_x/CeO_2NR catalysts with the 1:2 ratio of Co to Cu was confirmed to be the most effective for the oxidation of CO at low temperature. Besides, all the CeO_2NR supported cobalt-based bimetallic catalysts exhibited relatively high surface area (> 100 m^2/g) and excellent oxygen storage capacity (from 468.2 to 641.0 μmol g^{-1}). Additionally, investigation on the support effect proved that the reducible CeO_2NR with its unique reducible property and oxygen storage capacity, can show great promotion to the catalytic activity, in comparison with irreducible silica support.

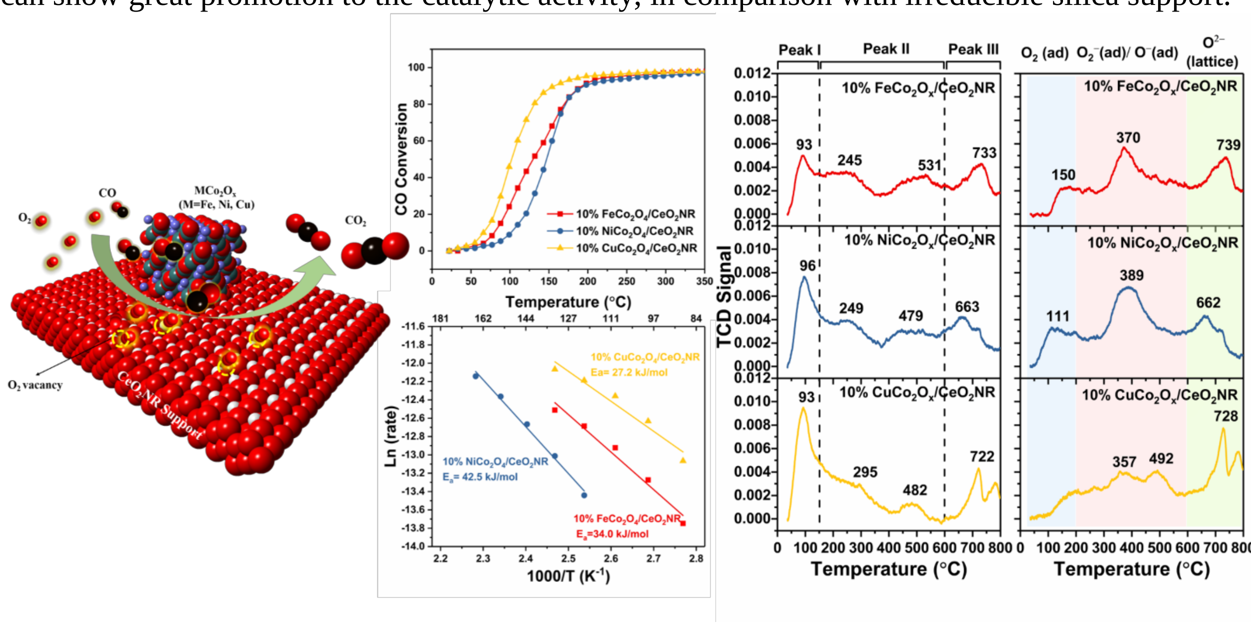

Fig. 1 Structural schematics (left), CO conversion (middle top), Arrhenius plots (middle bottom), CO-TPD and O_2-TPD (Right) of CeO_2NR supported MCo_2O_x (M=Fe, Ni and Cu) catalysts.

Plasma-Catalysis Chemical Looping CH_4 reforming with water splitting using ceria supported Ni based La-perovskite nano-catalyst

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Chemical Looping reactions have the advantage of producing useful chemicals, with minimal energy penalty while achieving Carbon Capture Sequestration (CCS). We present the results of Plasma Catalytic (PC) CH_4 reforming reduction cycle coupled with PC water splitting oxidation cycle to produce hydrogen. We use CH_4+CO_2 flow reduction cycle with nano-powder, 50:50 mass ratio of $La_{0.9}Ce_{0.1}NiO_3$ perovskite with CeO_2 solid mixture as catalyst with Oxygen Carrier (OC) combination. The material is oxidized with H_2O+Ar during the oxidation cycle leading to H_2 production by water splitting. The primary goal is to study the plasma-assisted reforming and water splitting, with the purpose of achieving significant reactions at low temperatures (150-400 ᴼC). Significant water splitting H_2 production (24-30 µmole/g total) and CH_4 reforming (14-43 % conversion) was observed in 150-400 ᴼC temperature range, while no such reactions were observed without plasma in this low temperature range, with just the oxygen carrier nano-materials. Significant enhancements were also observed at higher temperatures.

Investigation of Pt-Zn Intermetallic Nanocatalysts for Oxidative Dehydrogenation of Ethane

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Light Alkenes such as ethylene and propylene, are important building blocks for many value added chemicals, including polymers (polyethylene, polypropylene), oxygenates (ethylene glycol, propylene oxide), and chemical intermediates (ethylbenzene). The demand for these building blocks is increasing with a 20% growth rate per 5 year Oxidative dehydrogenation (ODH) of light alkanes is a promising alternative to steam cracking because of its exothermal nature that requires less energy and it produces alkenes of higher purity. Pt is preferred in light alkane dehydration due to its affinity to paraffinic C-H bond over C-C bond. However, large Pt particles may cause side reactions such as hydrogenolysis and coke formation. Recent developments in alkane dehydrogenation pointed out that alloying Pt with other metals such as Sn, Cu, In, Zn may create Pt-based intermetallic alloy phases that suppress side reactions, due to their advantage in providing ordered structure with isolated Pt surface sites rather than solid solutions in which atoms are randomly arranged. In this work silica supported Pt-Zn intermetallic nanoparticles were synthesized. The relationship between structure and performance in ODH of ethane was established using synchrotron based in situ X-ray Absorption Spectroscopy (XAS).

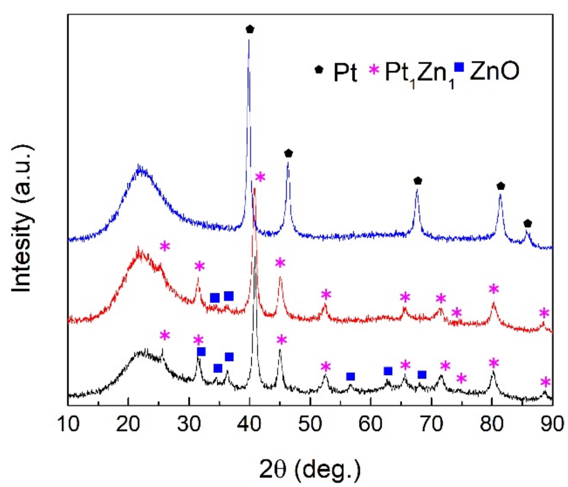

Figure. XRD patterns for Pt/SiO_2 (blue), $Pt/1cZn/SiO_2$ (red) and $1cZn/Pt/SiO_2$ (black).

Tunable Quasi-One-Dimensional Ribbon Enhanced Light Absorption in Sb_2Se_3 Thin-Film Solar Cells Grown by Close-Space Sublimation

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Abstract

Solar cells directly convert the sunlight to electricity and provide affordable and sustainable energy. Recently, thin film solar cells attract great attention due to its light-weight and flexible and high power conversion efficiency. Sb_2Se_3 is a promising absorber material to make thin-film solar cells because it is low-cost, non-toxic and earth-abundant. The theoretical maximum efficiency of Sb_2Se_3 can achieve ~ 32%, corresponding to its 1.1 eV bandgap based on the Shockey-Quessier limit. Particularly, the orthorhombic crystal structure of Sb_2Se_3 indicates a nonisotropic photoexcited carrier transport behavior. Thus, it is tunable to achieve grain orientation dependent device performance. Also, it is a challenge to deposit high-quality Sb_2Se_3 film due to it is non-cubic crystallinity. Close-space sublimation (CSS) is an ultra-fast physical vapor deposition technique (~1 um min^{-1}). Here, we employ the CSS growth technique to tune the growth behavior of Sb_2Se_3 and to realize a high quality Sb_2Se_3 thin film solar cells with high efficiency. This study paves the way to scale up the manufacturing of a type of new non-cubic absorbers with the quasi-one-dimensional ribbons.

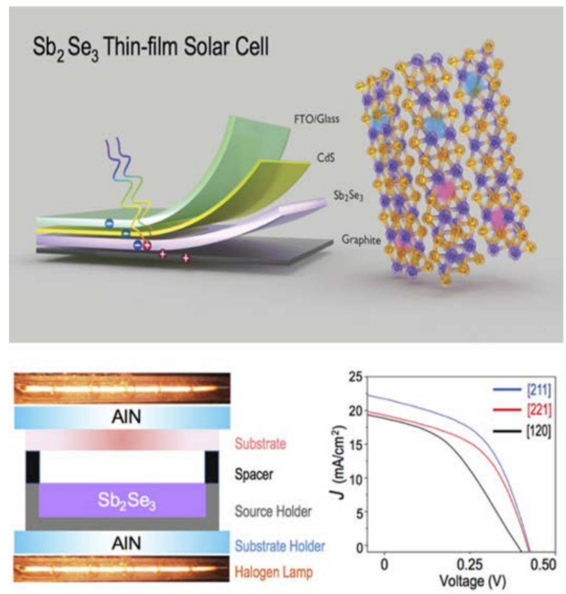

Figure 1 (Top)The solar cells structure of the CdS/Sb_2Se_3 devices. (Bottom, Left) Schematic of the CSS deposition technique, and (Bottom Right) The current-voltage curve as a function of $(Sb_4Se_6)_n$ ribbons oridentations

Session IV – Material Chemistry

Oral presentations

Challenges and Value in Atom Probe Tomography of Cementitious Materials

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Concrete represent the largest material usage in the world by mass. Such an important material for humanity warrants a holistic understanding of the material down to the atomic level. However, the poorly crystalline and heterogeneous constituent phases of the cementitious materials of concrete limit common experimental techniques such as X-ray diffraction. Atom probe tomography (APT) is a technique that is well developed for characterizing nanoscale heterogeneity in metallic and semiconductor materials. Recent advances in the laser pulsing capabilities of APT equipment has enabled the analysis of less conductive materials like ceramics, minerals and even cement. This study uses APT to analyze a fly ash based geopolymer cement and brings light to some of the potential challenges of adapting traditional APT methods to the analysis of cementitious materials. This study also demonstrates that valuable information can be gleaned from APT of cementitious materials. Potential improvements and applications of APT for future research of cementitious materials are also identified

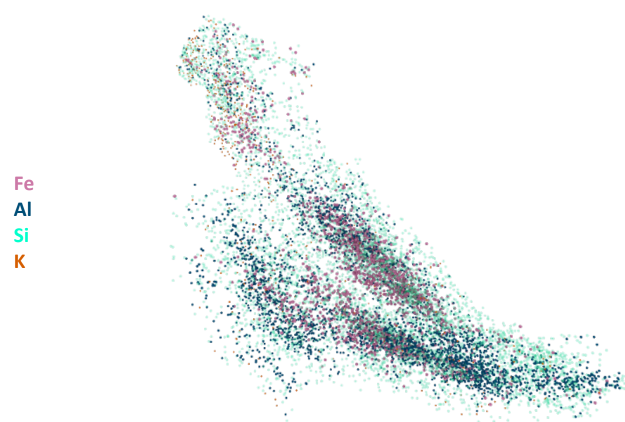

Figure 1. Atom probe tomography of an unreacted fly ash particle. Each sphere represents a detected ion.

Incorporating thermally stable ligands into hierarchically porous carbon.

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Fixed bed carbon catalysts are formed by adding metal salts to porous carbon. A new synthesis approach based on carbonization of porous polymer precursors opens up the possibility of making a hierarchically porous carbon incorporating metal ions and metal nanoparticles in a single reaction. The procedure for the synthesis of such catalysts employs a sol-gel method based on the formation of resorcinol-formaldehyde (RF) gel containing a transition metal complex and carbonizing at 500°C. The presence of Cu^{2+} species was monitored using electron paramagnetic resonance (EPR). Three types of Cu-complexes were studied, Cu-salen, Cu-protoporphyrin IX and Cu-phthalocyanines. The Cu-salen incorporated into the sol-gel polymer lost all EPR signal when heated to 200°C and lead to agglomeration into large copper nanoparticles when heated to higher temperatures. On heating to 380°C EPR of the Cu-protoporphyrin IX showed there was some complex present. EPR studies of the Cu-phthalocyanines dispersed in the RF gel, showed that after heating to 500°C the resulting carbon still contained significant amounts of the Cu-phthalocyanine complexes. Heating to 800°C showed the presence of some amount of Cu^{2+}. SEM images of the Cu-phthalocyanines incorporated in carbon showed only small numbers of metal nanoparticles indicating the presence of lower sized nanoparticles.

Oxime cross-linked alginate hydrogel threads with tunable stress relaxation

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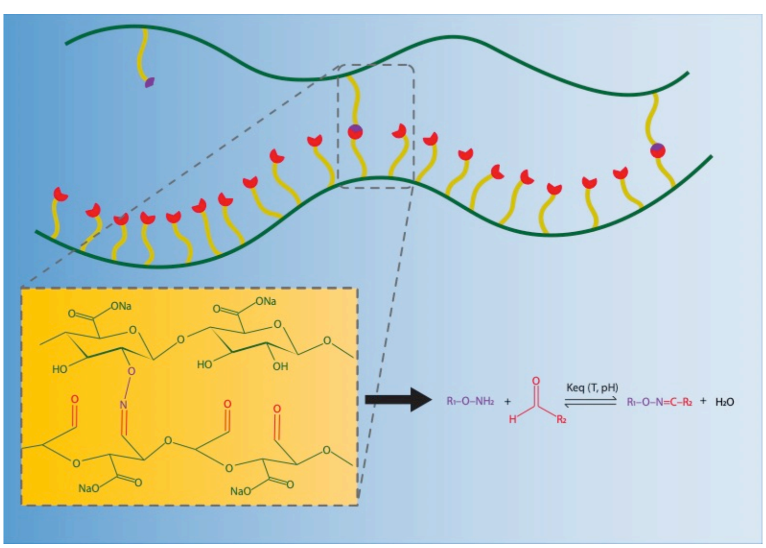
Abstract

Sodium alginate hydrogels have served as a versatile and reliable tool for biomedical applications such as 3-D cell encapsulation, both in vitro and in vivo. These hydrogels have formed via ionic or covalent cross-linking of the alginate chains upon the modification of its functional groups. Hereby, we employ a technique to modify hydroxyl groups of the alginate backbone to alkoxyamine groups. Alkoxyamine groups belong to the field of click biorthogonal polymer cross-linking. In the presence of aldehyde-modified alginate chains, both polymers can form an oxime reversible covalent crosslink, which has been proven to be environmentally responsive (pH and temperature). Upon hydrogel formation in physiologically relevant aqueous media (pH 7.4, 37ºC), gels of a wide variety of stiffnesses (storage moduli of G' = 80 Pa - 12 kPa) and stress relaxation capabilities can be achieved. These properties can be tailored by controlling the previously mentioned environmental variables, the overall polymer concentration of the hydrogel, the ratio between alkoxyamine and aldehyde groups, and the degree of functionalization of the aldehyde-alginate counterpart. Here, we employ an electrojetting extrusion technique to form hydrogel threads with a diverse set of viscoelastic properties.



Scheme of oxime cross-linking of alginate chains.

Session V - Bio/organic materials

Oral presentations

Three-dimensional hyaluronic acid hydrogels to investigate glioblastoma stem cell behaviors

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Abstract

Polymeric hydrogels have been extensively employed to study cancer cell-matrix interactions as they provide a relevant three-dimensional (3D) context evidenced *in vivo*. Herein, we utilized hydrogels composed of hyaluronic acid (HA), a glycosaminoglycan predominantly found in the brain microenvironment, to study glioblastoma stem cell (GSC) behaviors. Glioblastoma multiforme (GBM), the most common type of brain tumor in adults, is extremely malignant and lethal. GBM tumors are composed of tumor cells and GSCs that contribute to drug resistance and tumor recurrence following surgery. To improve drug efficacy, targeting GSCs and their microenvironment appears to be a promising approach. HA hydrogels were engineered to mimic the stiffness noted for brain tissue and were used to encapsulate cancer cells. Specifically, U87 cell line grown adherently (with serum) and as suspension culture (serum-free), and patient-derived D456 cells were used. We observed that these cells were able to form spheres, and sphere size increased over 14 days in the hydrogels. Increase in sphere sizes over time indicated proliferation of cells in the hydrogels. Also, U87 and D456 cells grown as suspension culture retained their expression of stem cell markers in HA hydrogels. Overall, such systems could further our understanding of microenvironmental regulation of GSC phenotype.

Impact of quinic acid and tannic acid surface functionalization on the uptake of ultrasmall iron oxide nanoparticles by cancer cells

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Abstract

Ultrasmall iron oxide nanoparticles (USIONPs) have recently attracted significant attention because of their potential as positive T_1 MRI contrast agents. This makes USIONPs a potential platform for cancer diagnostics and therapeutics. The diagnostic and therapeutic efficacy of USIONPs is determined by the cellular uptake. However, the impact of physico-chemical properties of USIONPs on the cellular uptake is relatively less known. In order to address this issue, we specifically investigated the role of USIONPs surface functionalities (tannic acid (TA) and quinic acid (QA)) in mediating cellular uptake behavior of cancer cells pertaining to primary (U87) and metastatic (MDA-MB-231Br) brain malignancies. We observed differential cellular uptake in case of TA and QA coated USIONPs by cancer cells. Cancer cells showed significantly higher cellular uptake of QA coated USIONPs compared to TA coated USIONPs at 4, 24 and 72 hr. Detailed characterization suggested that P-selectin cell surface receptors played an important role in the cellular uptake of QA coated USIONPs. Given that P-selectin is overexpressed in cancer cells, tumor microenvironment and at the metastatic niche; QA coated USIONPs hold potential to be utilized as a platform for tumor-targeted drug delivery and in imaging and detection of primary and metastatic tumors.

Rapid Diagnostics of Mycobacteria with Lectin Conjugated Silica Coated Magnetic Nanoparticles

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Development of a fast, rapid and sensitive bacterial determination method is crucial in medical diagnostics. Tuberculosis is caused by bacteria *Mycobacteria tuberculosis* (Mtb) is a highly contagious illness causing approximately one million deaths per year. Current methods of Mtb detection are time-consuming, labor intensive and expensive. We have developed a rapid diagnostic method of detecting Mycobacteria using lectin conjugated silica coated magnetic nanoparticles (SMNPs). The lectin Concanavalin A (ConA) and Aleuria Aurantia Lectin (AAL) recognize the mannose and arabinose carbohydrate epitopes found in the cell wall of the Mycobacteria. The multivalent Con A/AAL conjugated SMNPs bind to the bacterial cell wall and crosslink the bacteria within minutes to form a visible precipitate without the need of any instrumentation. Control studies were done with orally abundant cross contaminating microorganisms such as *Streptococcus mutans* and other non-binding proteins such as Wisteria Floribunda Lectin (WFL) and Bovine Serum Albumin (BSA). SMNPs conjugated with Mtb polyclonal antibodies are used to compare the binding efficiency of Con A and AAL conjugated SMNPs.

Session VI – Nanomaterials

Oral presentations

Study of the Potential Energy Landscape of the different Grain Boundary phases of Cu-Zr Nanocrystalline Alloy

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The nanocrystalline alloy is currently one of the most exciting and prosperous areas of mechanical engineering and materials science research due to the promise of exceptional performance when characteristic microstructural length scales are in the nanometer range. Segregation induced structural transitions at grain boundaries of nanocrystalline alloys are studied using hybrid Monte Carlo/Molecular dynamics simulations in a Cu-Zr model system. Complexion transitions are simulated at different temperatures with increasing Zr doping in nanocrystalline Cu. With increasing the global composition, the thickness as well as the composition in the grain boundary increases, and the initially formed ordered complexions transform into the disordered complexions. The grain boundary structure of different phases is characterized by a radius distribution function, Voronoi analysis, giving atomic details on the structural transition. The activation-relaxation technique (ART) is used to identify the transition (saddle) state and spectrum of activation energies and explore the grain boundary energy landscape for both ordered and disordered phases. The simulated results are used to construct the grain boundary phase diagram, providing a guideline for experiments on synthesizing nanocrystalline alloys.

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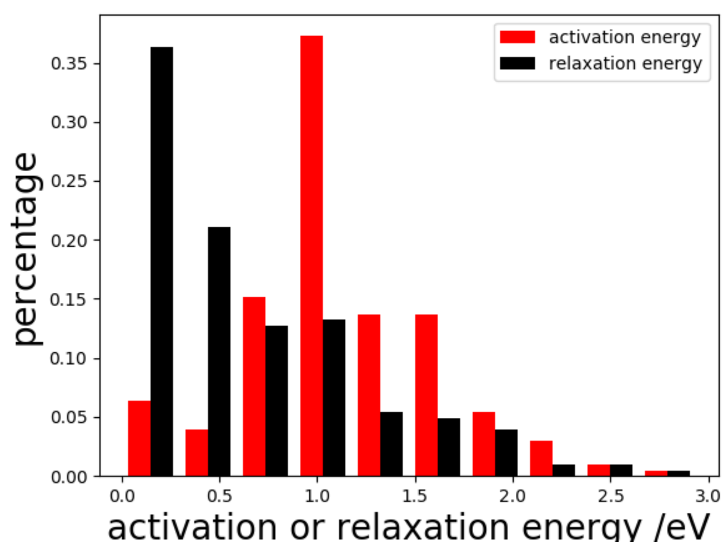

Figure 1. Activation and Relaxation energy distribution of ∑5 (310) Cu-bicrystal using ART.

Chemical composition tunes the nanoscale heterogeneity in metallic glass thin films

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The inherent nanoscale heterogeneity of metallic glass is investigated in the CuZr alloy system with various compositions. The co-sputtering method with two single targets (i.e., Cu and Zr) is employed to control the composition, during which the deposition power and pressure are tuned individually. The X-ray diffraction results confirm the amorphous structure of the thin films. The topography, non-contact mode amplitude, and phase shifts are spatially resolved by atomic force microscope for inelastic performance. Based on the characterizations, the glass forming ability, viscoelastic properties are analyzed to explore the connection between the performance and chemical composition.

Organic Additives in Deposition of Cobalt for Advanced Interconnects

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The concerns about copper (Cu) interconnects have been increasing because the Cu line resistance will not linearly scale with the dimension in 7 nm technology and beyond. Instead, Cu resistivity in small features increases significantly because of the electron scattering at grain boundaries and interfaces. To solve this problem, alternative metals such as cobalt (Co) is considered as a promising material because of its high melting point and small mean free path. High melting temperature lows the risk of electromigration and small mean free path decreases the contribution from electron scattering at boundaries and interfaces. Different functional groups in organic additives were found to influence Co electrodeposition kinetics. For instance, additives with a conjugated pair of oxime groups displayed strong suppression effects on Co deposition and a suppression breakdown occurs upon the reduction of adsorbed Co-dioxime chelates. This talk presents a study, where we used several dioxime additives like dimethylglyoxime (DMG), cyclohexane dioxime (CHD), and furil dioxime (FD) to investigate their impacts on Co nucleation process.

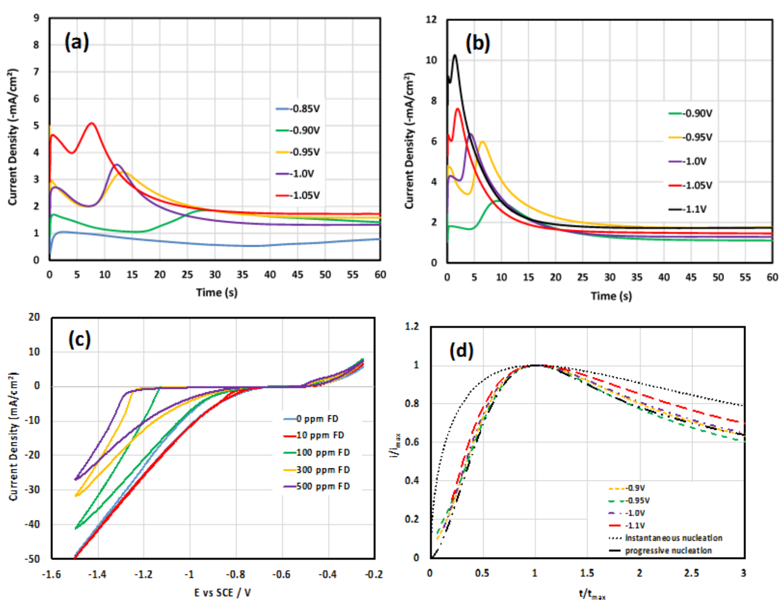

Fig. 1 (a) Co nucleation process with the addition of 100 ppm DMG (b) Co nucleation process with the addition of 10 ppm CHD (c) The CV results with the addition of different concentration of FD (d) Normalized current transients with 10 ppm FD.

Epitaxial Al films for superconducting resonators

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Superconducting resonators fabricated from aluminum thin films are shown to have high quality factors ($>10^6$). However, unexpected losses are theorized to come from poor metal-substrate interface or crystallinity. We have grown epitaxial aluminum film on c-plane sapphire using DC magnetron sputtering with varying growth and prebake temperatures and pressures, along with various substrate preparation. We found that an in situ pre-growth substrate anneal in 20mTorr O_2 results in Al films with good crystallinity and smoothness, while minimizing void and pinhole defects.

Gallium-Based Liquid Metal Alloys for Use in Stretchable Electronics and Soft Robotics

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Gallium-based room-temperature liquid metals present an exciting opportunity in the fields of stretchable electronics and soft robotics due to their unique properties such as high electrical and thermal conductivity, low toxicity, and intrinsic deformability. These liquid metals are mechanically stabilized by a native oxide layer which forms on their surface upon exposure to oxygen. Manipulation of this oxide layer can lead to a desired shape or flow of the liquid metal as well as unique surface chemistries. We are interested in understanding the novel electronic properties that could be imparted to a stretchable device by these liquid metal oxides. The work presented will display the results of characterization experiments performed on the oxide layer such as x-ray photoelectron spectroscopy (XPS), energy dispersive x-ray spectrometry (EDS), x-ray diffraction (XRD), and Raman spectroscopy. These experiments have led to a greater understanding of the molecular and elemental composition, crystal structure, and surface homogeneity of the oxide layer. Liquid metals as a deformable conductive element for stretchable electronics and effective use of their native oxide have the potential to dramatically impact soft, stretchable electronic production and capabilities.

Improve the Stability of Organic-Inorganic Hybrid Perovskite by Atomic Layer Deposition

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Organic-inorganic hybrid perovskites, such as $CH_3NH_3PbI_3$ and $NH_2CH{=}NH_2PbI_3$, emerge as a new class of low-cost semiconductors that has the potential to revolute the fields of high efficiency photovoltaic cells, light emitting diodes, lasers and sensors. However, hybrid perovskites have poor stability as they can be easily degraded by H_2O, O_2, and light in ambient conditions. Atomic layer deposition (ALD) is a promising method to improve their stability by depositing a pinhole-free metal oxide barrier film onto perovskites. This thin pin-hole free barrier layer can not only block H_2O and O_2 from meeting perovskites, but also encapsulate the gas byproducts from the degradation reactions to stop the reversible degradation reaction. Although there are numerous reports in applying ALD on hybrid perovskites, the mechanism of nucleation of ALD on these perovskites are poorly understood. Herein, we will present our new findings about the atomic level surface reaction mechanism during ALD on perovskite related substrates. We explore the reaction mechanisms during ALD on perovskite related substrates by using *in situ* quartz crystal microbalance, infrared, and quadrupole mass spectrometer. Collectively, we are able to create a couple of new pathways to improve the stability of perovskite materials.

Poster Presentations

Magnetic Materials

#1 Influence of preparation method on the morphology of magnetic $CuCr_2Se_4$ nanoparticles

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$CuCr_2Se_4$ is ferromagnetic chalcospinel with the Curie temperature of 430K that makes this system interesting to study among the ternary metal-chalcogenides. Herein, we have reported two colloidal synthesis strategies based on thermal decomposition of the $CuCl_2$ and $Cr(acac)_3$ precursors in the presence of selenium and we discussed the influence of the preparation method on the shape, size, and morphology of the products. The prepared nanoparticles were characterized by XRD and their morphology has been studied by TEM. The $CuCr_2Se_4$ nanorods were selectively synthesized in a one-pot heat-up reaction at 330 °C by using the reagents and octadecylamine (ODA) as the capping agent. Whereas rapid hot injection of the mixture of Cu- and Cr-precursors into the Se-ODA solution at 330 °C led to the formation of triangular and hexagonal $CuCr_2Se_4$ nanocrystals.

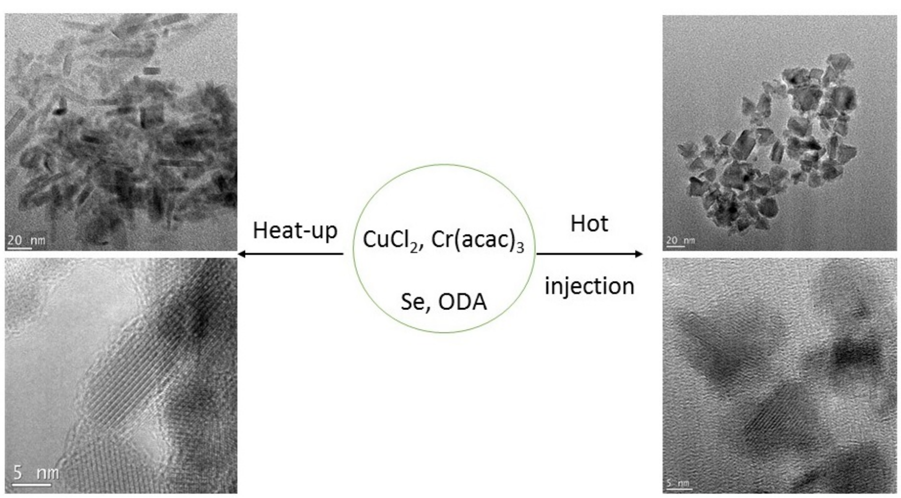

Fig. 1. TEM and HRTEM images of $CuCr_2Se_4$ nanocrystals formed by heat-up and hot injection methods.

#2 Structural, Magnetic and Mechanical Properties of $Co_{2-x}Ti_xFeGe$ ($0 \leq x \leq 1$) Alloy Series

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Abstract

Structural, magnetic and mechanical properties change with the addition of Ti, by replacing Co atoms in Co_2FeGe Heusler alloy have been investigated. From the bulk synthesis of $Co_{2-x}Ti_xFeGe$ ($0 \leq x \leq 1$) alloy series in steps of $x = 0.125$, we report single phase behavior for $0.125 \leq x \leq 0.625$, while the rest showed multi-phase microstructure. The lattice parameter was observed to scale linearly with the Ti concentration attributed to the larger atomic radii of Ti than that of Co atoms. Similar linear behavior was observed for extracted saturated magnetic moment. Moreover, the experimental low temperature saturated moment agreed well with the Slater-Pauling moment indicating the presence of possible half metallic behavior in the samples. The theoretical calculations performed agreed well with the experimental finding, predicting a half-metallic behavior in case of $Co_{1.5}Ti_{0.5}FeGe$. In addition, the hardness test was carried out using Vickers micro indenter and considerably high hardness values were obtained. The hardness was also observed to climb up with the Ti concentration.

#3 Vectorial observation of the spin Seebeck effect in epitaxial $NiFe_2O_4$ thin films with varying magnetic anisotropy

Zhong Li[1,2], Jan Krieft[3], Amit Vikram Singh[1], Sudhir Regmi[1,2], Ankur Rastogi[4], Abhishek Srivastava[1,2], Zbigniew Galazka[5], Tim Mewes[1,2], Timo Kuschel[3], and Arun Gupta[1]

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A vector measurement of the spin Seebeck effect (SSE) in epitaxial $NiFe_2O_4$ thin films has been developed. The $NiFe_2O_4$ thin films are grown by pulsed laser deposition on (011)- or (001)-oriented $MgGa_2O_4$ and $CoGa_2O_4$ substrates with varying lattice mismatches. We confirm that a large lattice mismatch leads to strain anisotropy in the thin films using vibrating sample magnetometry and ferromagnetic resonance measurements. Moreover, we show that the existence of a magnetic strain anisotropy in $NiFe_2O_4$ thin films significantly impacts the shape and magnitude of the SSE voltage hysteresis loops. We further demonstrate that voltage signals from bidirectional SSE measurements can be utilized to reveal the complete magnetization reversal process, which establishes a new vectorial magnetometry technique based on the spin caloric effect.

#4 Tuning structural, magnetic and mechanical properties by vanadium substitution in Fe_3Ge

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The structural, magnetic and mechanical properties of V-substituted Fe_3Ge, i.e., $Fe_{3-x}V_xGe$ intermetallic alloy series ($0 \leq x \leq 1$) have been investigated. Novel polycrystalline intermetallic alloys were prepared by arc-melting under argon atmosphere. After annealing, alloys for $0.375 \leq x \leq 0.75$ are found to crystallize in the cubic Heusler structure, while alloys with $0 \leq x \leq 0.25$, crystallize in the hexagonal DO_{19}, which is the high temperature structure of the parent Fe_3Ge. Higher V concentrations ($x > 0.75$) are multi-phased. Optical microscopy, SEM/EDX, and XRD reveal uniform granular microstructures without any secondary phases for $x \leq 0.75$. The calculated lattice parameter increases linearly with increasing V concentration for cubic alloys, while the magnetic moment at 5K decreases linearly with V concentration, deviating only about ~6% from the expected Slater-Pauling values, which indicates possible half-metallic behavior. The hexagonal samples have markedly higher moments. The saturation magnetizing field is found to decrease with the increase of vanadium concentration making the system softer at higher vanadium concentrations. The martensitic phase transformation in all stable cubic phases is confirmed by DSC. Vanadium is found to play a crucial role in changing the mechanical properties, stabilizing the cubic structure and shifting the martensitic transformation temperature to higher values from that of parent Fe_3Ge.

#5 Low Temperature Broadband Ferromagnetic Resonance measurements on NiFe/Cu/IrMn/CoFe exchange biased system

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We performed low temperature ferromagnetic resonance measurements of exchange biased NiFe/Cu/IrMn/CoFe multilayers. In this sample structure we are able to investigate the influence of the exchange bias effect of the CoFe/IrMn bilayer on the magnetization dynamics of the NiFe layer. Ferromagnetic resonance experiments were carried out with the static external field parallel and antiparallel to the exchange biased direction. In the antiparallel configuration we observe a pronounced peak in the linewidth when the applied field is able to reverse the pinned CoFe layer. This linewidth enhancement is hysteretic, i.e. it depends on the field history of the sample and is consistent with an inhomogeneous broadening of the resonance of the NiFe layer due to the stray field emanating from domains formed in the CoFe layer during reversal. These results highlight the importance of long range dipolar interactions in multilayer thin films for the magnetization dynamics and show how they can be used to tailor the high frequency properties of materials.

#6 Growth of spinel ferrite $NiFe_2O_4$ on lattice matched substrates

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Spinel ferrite thin films have been widely studied from the past few decades because of their potential use in microwave and high frequency device applications. These materials possess low coercivity, high saturation magnetization and high remnant magnetization, and magnetic properties are less sensitive to high frequency environment. Here, we report the synthesis and detailed characterization of spinel ferrite $NiFe_2O_4$ (NFO) thin films grown by pulsed laser deposition (PLD) technique on the range of isostructural substrates from $MgAl_2O_4$ (~ 3% mismatch), $MgGa_2O_4$ (~ 0.7% mismatch) to closely matched $ZnGa_2O_4$ (~ 0.07% mismatch). The result of X-ray diffraction (XRD) analysis and reciprocal space mapping (RSM) confirmed the bulk-like strain free film on less lattice mis-matched substrate which in turn exhibits low strain anisotropy on the film. Magnetometry results from vibrating sample magnetometry (VSM) supports the two antiferromagnetically ordered spin sublattices structure of NFO. Furthermore, these films also exhibits very low Gilbert damping parameter of $\alpha \sim 0.0016$, as result of small inhomogeneous linewidth broadening(ΔH_o) and low linewidth of $\Delta H \sim 19$ Oe at the frequency of 10 GHz.

#7 The Influence of Composition on Chemical Partitioning and Partial Crystallization Behavior in CoFeMnSiBNb Soft Magnetic Materials

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Abstract

Partially crystallized soft magnetic alloys can exhibit tunable permeability based on composition and annealing treatments. By varying the Mn-to-Co content in a CoFeMnSiBNb alloy, the permeability can be substantially increased with decreasing Mn content. To study this effect, 0.5 to 6.0 at. % Mn was systematically changed with the annealing fixed at 520 deg. C for 20 minutes to promote crystallization. Atom probe tomography was used to quantify the chemical partitioning behavior between the amorphous and crystalline phases. It was found that Co partitioned strongly to the crystalline phase, with Fe's partitioning to this phase increasing with Mn content. This poster will discuss the role of Mn in assisting in Fe enhanced partitioning and its effects on the magnetic properties for this alloy.

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POSTER PRESENTATIONS

Advanced Manufacturing Materials

#8 In-Situ 3-D metal printing using locally sourced material

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Abstract

As the exploration of outer space continues, the need for structural components produced in-situ from locally available resources is an increasing concern. Iron can be chemically extracted from material such as lunar regolith and recovered as flakes of nearly pure metal. These flakes can then be processed and used in a blown-powder application to 3-D print Iron or steel components.

Ferritic iron has been extracted from a meteorite using a method which could also be applied to lunar regolith. This metal has been characterized and will be simulated using chemically pure iron powder. Further processing will be explored to demonstrate the suitability of blown-powder 3-D printing to form components from this material. It is the goal that this method will be a stepping stone to producing structurally robust components in the low gravity vacuum of space.

#9 Microstructural and Mechanical Behavior of High-Shear Solid-State Deposition of Rare Earth Magnesium Alloy WE43

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Abstract

A transformative hybrid solid-state additive manufacturing process, Additive Friction Stir Deposition (AFS-Deposition) provides a new path to either fabricate or repair components for wrought performance. In this work, the fatigue behavior of AFS-Deposition manufactured Inconel 625 is characterized and modeled. The AFS-Deposition method is a unique solid-state manufacturing process that differs from traditional friction stir welding since solid rod is fed through a non-consumable rotating cylindrical tool generating heat and plastically deforming the feedstock material through controlled pressure as successive layers are built upon a substrate. In order to quantify the fatigue behavior of the AFS-Deposition Inconel 625, strain-life experiments were conducted under low and high cycle conditions. The cyclic behavior of this alloy displayed varying degrees of cyclic hardening depending on the strain amplitude. However, AFS-Deposition Inconel 625 appeared to exhibit generally superior fatigue performance compared to the wrought Inconel 625.

#10 Laser Assisted Cold Spray of Ferritic Alloys

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This poster will show the results for cold spray deposition of laser assisted cold spray (LACS) for the consolidation of ferritic powders. Cold spray deposition is widely applied to additive repair and manufacturing of metallic components, but the deposition efficiency of hard materials is low because of the powders' inability to undergo sufficient deformation upon impact. Here, LACS was demonstrated to successfully deposit ferritic powders into a consolidated material. ODS $Fe_{91}Ni_8Zr_1$ powders, containing nano-scale zirconia clusters, and AISI 4340 were deposited under various laser powers up to 1kW. The laser provided *in situ* heating and resulted in a 100% increase in deposition efficiency. In the case of the ODS alloy, heating from the laser increased the ferrite grain size from 2µm to 7µm. The dispersed oxide particles survived LACS and increased slightly in size. These changes in microstructure and nanostructure resulted in a measurable reduction in hardness with increasing laser power.

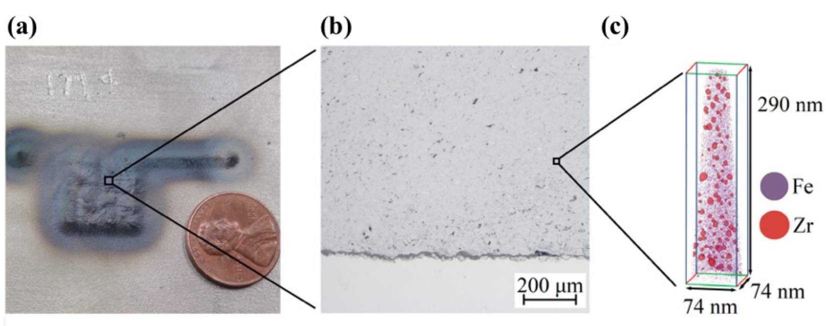

Figure 1: (a) LACS deposit of ODS $Fe_{91}Ni_8Zr_1$ with **(b)** an accompanying micrograph of the deposit and substrate and **(c)** atom probe tomograph demonstrating the presence of ZrO_2 clusters still present in the material.

#11 Meshfree Simulation of Oxide Dispersion in MELD of Aluminum Alloys

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The MELD process (formerly additive friction stir deposition) is a solid-state process in which the feedstock material is deposited on the substrate via a hollow rotating tool. As it flows through the rotating deposition tool, the feedstock material undergoes severe plastic deformation and dynamic recrystallization. While wrought-like properties are achievable through MELD, defective deposition can occur due to several factors including poor oxide film dispersion. Numerical modeling of the MELD process can be used to increase productivity and reduce the time needed to determine the operating window of the process. In this work, the MELD process is modeled using a mesh-free coupled thermomechanical approach called Smoothed Particle Hydrodynamics (SPH). Because of the Lagrangian nature of the meshfree method, the simulation model can readily track the dispersion of the oxide layer within the solid-state additively manufactured aluminum alloy part.

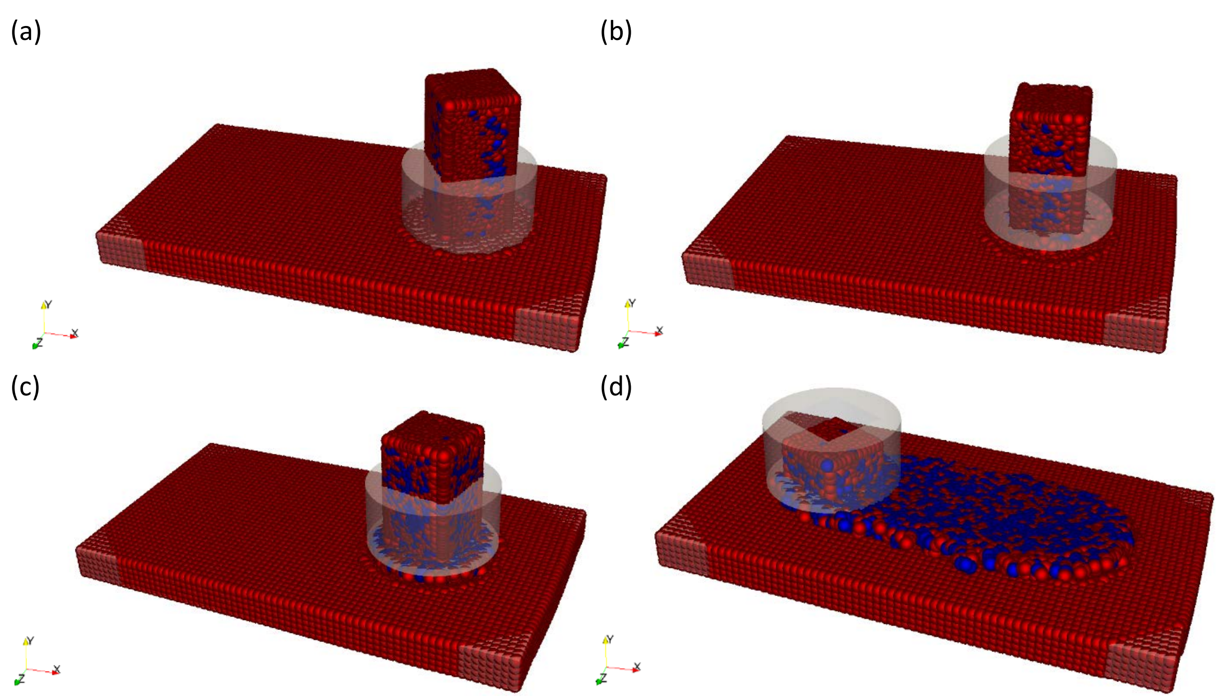

Figure 1. Oxide Dispersion of MELD Stages: (a) Dwell (b) Lift (c) Fill (d) Advance

Red = Oxide Layer; Blue = Aluminum Alloy

#12 Microstructure Evolution of Additively Manufactured Inconel 718

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Inconel 718 is a nickel-based superalloy that is of interest within the Additive Manufacturing (AM) field. The alloy has applications where retention of strength and corrosion resistance at elevated temperatures is required. While much research has been done to develop processing standards for wrought Inconel 718 produced under equilibrium conditions, optimization of AM Inconel 718 requires an understanding of the microstructural response to the inherent non-equilibrium conditions. The non-equilibrium conditions affect the elemental partitioning at various temperatures and times. After solidification, segregation of Niobium (Nb) from the matrix (γ) may lead to the formation of laves and delta phases which are detrimental to the mechanical properties. The following presentation aims to discuss these behaviors and expected phase formations in as-built AM structures and how they respond to post processing heat treatments. The experimental characterization of this evolution is modeled using first principles and data science techniques. To validate this modeling approach, Inconel 718 specimens were processed using powder bed fusion. X-ray diffraction (XRD) and transmission electron microscopy (TEM) were used to characterize the phase evolution at various post processing heat treatment stages of the PBF AM specimens.

#13 The As-Deposited Properties of Ti64 by High Shear Solid State Deposition

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MELD is a novel solid state additive manufacturing process used to produce parts from a vast selection of metal alloys. One such alloy is the titanium alloy Ti-6Al-4V (Ti64). Ti64 is the most widely used titanium alloy, used most often in the medical and aerospace fields. This titanium alloy is desirable for its high strength-to-weight ratio and corrosion resistance, but is comparatively much more expensive than aluminum or steel alloys. MELDing Ti64 saves time and money compared to conventional machining, where a majority of the material is turned into scrap. This research analyzes properties of Ti64 processed by MELD, such as ultimate tensile strength, hardness, and microstructure. These results are then compared to properties of Ti64 processed by other manufacturing methods, such as SLM, EBM, and DED. Due to the severe plastic deformation employed by this process, MELD Ti64 possesses equiaxed grains with an average size of less than one micron. For comparison, powder bed methods such as EBM and SLM produce columnar grains that range from 4-100 microns in size. The equiaxed microstructure of MELD Ti64 contributes to its exceptional as-built properties, which outperforms Ti64 produced by other popular manufacturing processes.

#14 Utilizing Ultrasonic Thermometry in Friction Stir Welding

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Abstract

Friction stir welding (FSW) is a solid state welding process that thermo-mechanically joins two metals. A rotating tool is plunged into the faying surfaces of a butt weld configuration and stirs the plasticized metal together. Heating of the metal occurs by friction of the tool against the material and the heat of deformation. If reliable methods to measure temperature can be demonstrated, this can become the basis for feedback control of the FSW process. While the quality of a FSW is dependent on maintaining a constant temperature, measuring the temperature can be difficult. Methods like thermocouples can compromise the tool integrity if embedded within the tool or run the risk of being consumed if placed within the weld path. Thermal imaging of welds can also prove challenging due to low emissivity of the material and changing surface reflectivity of the workpiece. Ultrasonic thermometry utilizes the change of material properties from temperature fluctuations to remotely capture temperature data. Ultrasonic thermometry has been demonstrated to be able to obtain the real time temperature profile within the weld zone. The method is non-invasive and can be adapted to move with the FSW tool to obtain continuous temperature measurements through the workpiece thickness.

#15 Effect of low temperature heat treatments on the resulting microstructure of blown powder deposition, additive manufacturing Inconel 625 specimens

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Abstract

In this study, specimens were obtained from four vendors using blown powder deposition (BPD) additive manufacturing processing of Inconel 625. Since Inconel has been used in various applications as a structural member in bi-metallic Ni to Cu components, its response to heat treatments at temperatures compatible with the Cu alloy must be understood. In addition to understanding the microstructural evolution of the Inconel at post processing temperatures compatible with Cu alloys, these experiments also evaluated variations in the response of additively manufactured Inconel 625 parts provided by four vendors. The specimens obtained were characterized using void analysis, microhardness testing, and grain size measurements before and after heat treatments. Three specimens from each vendor were subjected to different heat treatment temperatures of 950°C, 1000°C, and 1050°C. Specimens were removed in two orientations, the build plane and build direction, for each AM specimen. The void analysis of each unetched specimen was performed using optical microscopy. After the void size analysis, the specimens were etched to characterize the grain size and degree of recrystallization. To understand potential differences in mechanical properties, microhardness test was used to determine the variance in the relative hardness of Inconel 625 BPD specimens from different vendors.

#16 Process Parameter Microstructure Relationship for Solid State Additive Manufactured Aluminum Alloy 6061

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The Solid-State Additive Manufacturing MELD process provides a new path for coating, joining an additively manufacturing materials such as Aluminum Alloy 6061 (AA6061). This research is the first of its kind to investigate the process parameter relationship to the quality of MELD deposits. The process employs powder or solid rod is fed through a non-consumable rotating cylindrical tool generating heat and plastically deforming the feedstock material through controlled pressure from the tool as successive layers are built upon a substrate. Microstructural analysis characterized the dynamic recrystallization and grain refinement in successive layers in as-deposited samples using Electron Backscattered Diffraction (EBSD). The EBSD results depict grain structures formed by dynamic recrystallization (DRX) with even finer grains observed in the as-deposited material than the wrought filler material. Additionally, a fully dense equiaxed grain morphology is observed in the as-deposited structure. TEM analysis finds that the deposit dissolved strengthening precipitates typically inherent in the wrought material. Results from this work feed into continuing work to optimize the new process.

#17 Fatigue and Fracture of Solid-state Additive Manufacturing of Aluminum alloy 6061

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The solid-state Additive Friction Stir Deposition process, commercially known as MELD, is a novel additive manufacturing technique that works by depositing thin layers of material through a hollow, a rotating tool that stirs the material and achieves metallurgical bonding. The MELD process is a solid state process that results in fully dense builds with refined microstructure. In this work, the microstructure of MELD AA6061 is investigated and compared to that of a similar feedstock. In addition, monotonic and fatigue tests are carried out to determine the effect of MELD on the mechanical behavior of AA6061. Fatigue tests were conducted under strain control conditions. Fatigue of MELD material shows promise due to the lack of porosity commonly found in additively manufactured material. Post mortem analysis of the fracture was performed in order to determine the failure mode and well as the underlying microstructural damage mechanism.

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#18 Mechanical Properties and Microstructure of Carbon Fibers Deposited from Ethylene via Hyperbaric Chemical Vapor Deposition

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Carbon fibers were deposited from Ethylene in a laser chemical vapor deposition (LCVD) process at hyperbaric pressures. Equilibrium growth rate variation for different laser powers and precursor pressures was investigated. The influence of processing conditions on the mechanical properties and microstructure of the deposited fibers was also analyzed. It was found that deposition rates increase with laser power and precursor pressure but are restricted by the mass-transport limit. Fibers are comprised of a core-shell structure that evolves with processing conditions. Tensile strength increases with precursor pressure and is inversely related to laser power and growth rate. Sudden transitions in growth rate, mechanical characteristics and microstructure were observed at higher pressures.

#19 Influence of Process Parameters on Plasma Surface Modification

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Plasma surface modification has been extensive employed and is of great interest for biomaterials engineering. The influence of various processing parameters affects the degree and rate of surface functionality and has been demonstrated. Herein is described a plasma surface modification of an electrospun biomaterial (polycaprolactone) employing a radio-frequency inductively-coupled plasma (RF ICP) source operating at 13.58 MHz frequency, 45 W power, and 0.8 – 1.0 Torr pressure with ambient atmosphere as process gas introduced at 25 SCCM flow rate. The influence of both time and magnetization of the plasma is demonstrated. The magnetization increases the rate of surface modification with respect to unmagnetized plasma. A cobalt sample introduced into the chamber has an intermediate affect where presumably induced currents will produce a magnetic effect on the plasma modification rate. The influence of process time shows the most significant effects occurring in the early treatment times (< 5 mins) with all processes tending toward equilibrium at longer timescales.

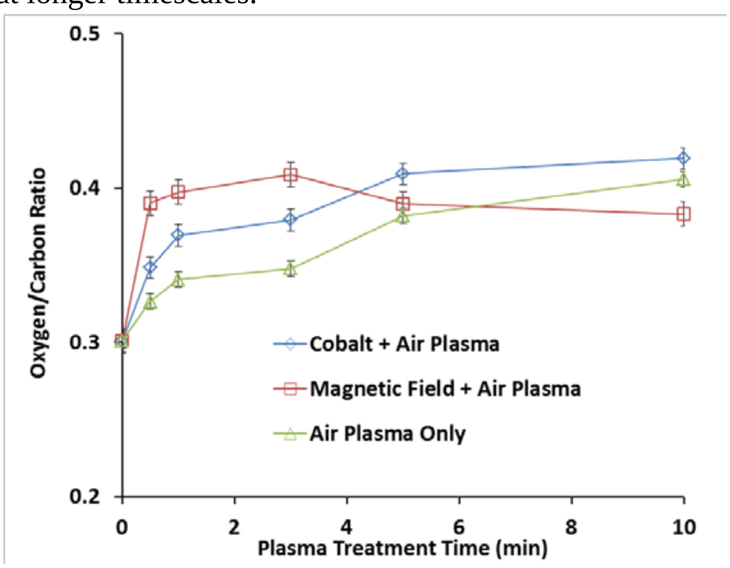

Figure 2. A comparison of the effects of magnetic fields, cobalt metal, in combination with air plasma is shown. The O/C ratios are reported as determined via x-ray photoelectron spectroscopy of the surfaces of the substrate. Error bars are standard deviation for n=3 for each measurement.

#20. Σ Forge: Low-Cost Open Source Prototyping and Research Platform

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Cost, consistent quality, and scalability associated with metal 3D printing in industry makes implementation a difficult prospect. Devices for metal printing can utilize various feedstocks including: wire, blown powder, or powder bed. Each method varies in cost, part build time, and feature resolution. Using open source hardware and software helps mitigate the cost while enabling the use of custom quality-control mechanisms. To design and fabricate this system, wire-fed was chosen due to the low cost associated with the process as well as the scalability of the system. Using open source software available for plastic 3D printers and a 3-axis CNC gantry system in conjunction with a MIG welder it was possible to achieve a highly cost-effective and scalable 3D metal printer. Implementation of a laser height sensor was added to increase the z-axis (or build direction) resolution. The low-cost testbed functionality of the Σ Forge allows for augmentations to be added for validating new printing methods, verifying transient thermal models, and acquiring data on specialized projects.

#21 The plastic strain and subsequent fatigue response of AA7050 friction stir welds

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This work examines the plastic strain gradients developed by pre-straining AA7050 friction stir welds (FSW), the damage to intermetallic particles caused by this strain, and the effect of these fractured particles on the subsequent fatigue performance of the weld. One particular application where pre-strained welds may be subjected to fatigue comes from the fabrication of stiffeners or multiple panels that are welded and then formed to shape. AA7050 FSWs were subjected to monotonic strains of 0%, 1% and 3%. The local plastic strain distribution was obtained by measuring the change in spacing between microhardness indentations before and after pre-straining. The plastic strain map shows the strain is concentrated in the HAZ, and that the maximum local strain is 3.34 and 1.83 times the average strain after 1% and 3% pre-strain respectively. Metallography from each pre-strain level shows that the fraction of cracked Mg_2Si and Fe-rich particles in the HAZ increases with increasing pre-strain. The strain life results show the 1% pre-strain group has lower life in HCF, while the 0% and 3% groups are virtually identical. Both Mg_2Si and Fe-rich particles were found at the initiation sites, with the 3% pre-strain group showing Fe-rich particles at 75% of the initiation sites. It is thought that after 1% pre-strain most of the damage to the particles has occurred, but only marginal work hardening. After 3% pre-strain however, the material has not only work hardened the area around the crack, but also the bulk sample, thus mitigating the effect of the cracked particle. Furthermore when correcting for the strain concentration, the maximum local strain vs. life curve for the 0% pre-strain FSW was found to match the base material very closely.

#22 Connecting Residual Stresses with Friction Stir Welding Conditions and Pseudo-heat Index

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This poster demonstrates the connections between friction stir welding (FSW) parameters, the simple pseudo-heat index (PHI) metric, and the resultant residual stresses on AA5052-H32 plates. Same PHI values in the range of 0.02 to 0.5 were achieved from combinations of different tool rotational speeds (283-1732 RPM) and tool traverse speeds (400, 600 MMPM). All of the friction stir welds produced the typical, M-shaped longitudinal residual stress profiles across the weld. The average residual stresses inside the stir zone increased from +80MPa to +133MPa as the PHI decreased from 0.5 to 0.02. The largest tensile stresses were observed for low PHI conditions, which did not fully consolidate the material and created a wormhole defect. For sound welds, the simple metric of PHI was not a good predictor of the stir zone residual stress; modifying FSW parameters such as increasing traverse speed with fixed rotational speed did systematically increase the residual stresses inside the stir zone. However, this study indicates that PHI is a valuable predictor of residual stresses on welds in the transition region between defective weldments and sound weldments.

#23 Corrosion Behavior of Aluminum Alloy AA7075 Cold Sprayed Coatings

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Abstract:
This presentation will discuss the corrosion behavior of cold spray deposited AA7075 coatings. Cold spray is often used to repair components damaged by corrosion, and so it is important to examine the corrosion behavior of the repair material and coatings. AA7075 deposits were produced using a high-pressure cold spray deposition system with helium gas. Helium-sprayed materials have very high density. The electrochemical characteristics of these deposits were measured in an immersed, artificial sea water environment. The helium-sprayed material was slightly less active than AA7075-T651 plate, with minimal indications of galvanic interaction from potentiodynamic polarization testing. Immersion testing in still water for three weeks showed classic pitting behavior for the helium-sprayed material with slightly less pitting than wrought plate.

POSTER PRESENTATION

Energy Materials

#24 Effects of TiO2 in Low Temperature Propylene Epoxidation Using Gold Catalysts

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Propylene Oxide is one the most important starting materials and chemical intermediate in the chemical industry that has a wide variety of usage. The current industrial production of propylene oxide is divided into two methods. They are i) The Cholorohydrin Process and ii) The Organic Hydroperoxide Process. The problem with these two is that the first one produces by-products which are harmful for the environment and the second one produces a co-product in a greater ratio than propylene oxide. Direct epoxidation with molecular oxygen has been proposed to be a green and alternative way to produce propylene oxide. Gold clusters in the nanometer range and isolated Ti active sites are considered to be highly selective for oxidation of propylene. Atomic layer deposition being a thin film deposition process holds a promising aspect in producing nano-catalysts. In this work a series of Au/TiO_2 /SiO_2 catalysts were prepared using atomic layer deposition and deposition method and studies were performed to establish a precise relation between the structure and the performance.

#25 CO oxidation over CeO_2 supported Ru nanoclusters: support shape and Ru valence state effects

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In this work, CeO_2 nanorods (NR), nanocubes (NC) and nanoctahedra (NO) were chosen to prepare supported Ru catalysts in order to investigate the correlation of the morphology and crystal planes of nanoscale CeO_2 support with their low-temperature CO oxidation activity. The 5Ru/CeO_2NR-r sample displays a superior low-temperature activity (~ 9% CO conversion at room temperature) among three different shaped 5Ru/CeO_2 catalysts after reduction treatment. The enhanced hydrogen consumption and CO conversion below 100 °C for the 5Ru/CeO_2NR-r sample indicates a strong Ru-CeO_2 interaction (i.e. the existence of Ru-O-Ce bond) which promotes the low-temperature reducibility of CeO_2 NR-supported RuO_x catalyst. From the results of XPS spectra, the dominant oxidized state Ru^{n+} species on the 5Ru/CeO_2NR-r sample suggests Ru ions diffused into CeO_2 lattice or the formation of Ru-O-Ce bonds at the interface through strong metal-support interaction. The concentration of oxygen vacancy defects on the 5Ru/CeO_2NR-r sample is significantly higher than those on the other two samples, which are essential for absorption/dissociation of oxygen molecules during CO oxidation reaction. The enriched surface defects on the exposed {111} planes of CeO_2 NR support contribute to the cationic ruthenium species formation, which is vital important for the superior low-temperature activity of CeO_2 NR supported RuO_x catalysts.

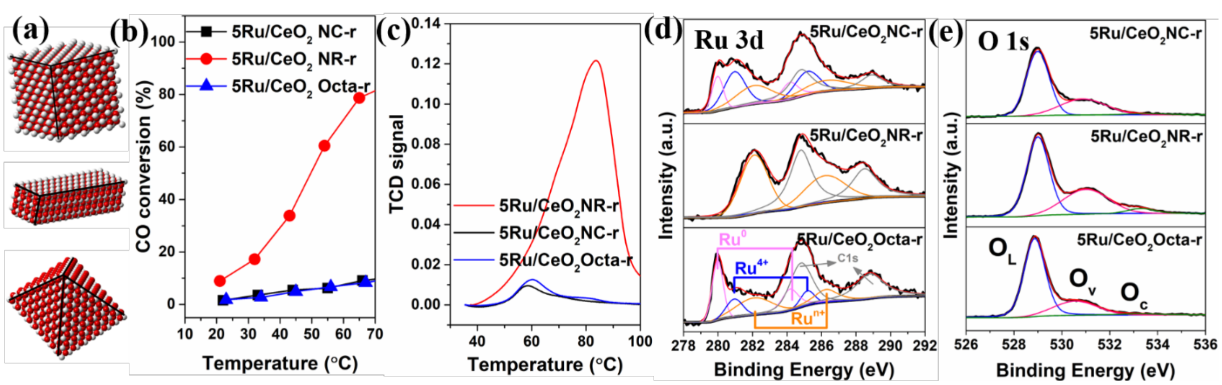

Figure 3(a) Crystal structure models of CeO_2 NC, NR and NO, (b) and (c) CO oxidation and H_2-TPR performance of different shaped 5 wt.%Ru/CeO_2 catalysts after reduction treatment, (d) and (e) XPS spectra of Ru 3d and O 1s.

#26 Solution-Processed Copper (I) Thiocyanate (CuSCN) for Highly Efficient CdSe/CdTe Thin Film Solar Cells

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Solution-processed CuSCN serves as a hole transport layer (HTL), an electron reflecting layer (ERL) and as a Cu dopant source for CdSe/CdTe thin-film solar has been developed with a high power conversion efficiency (PCE) of ~ 17%. Two types of solvents were used for the fabrication of CuSCN, diethyl sulfide (DES) and aqueous ammonia (NH_4OH), both with the ability to enhance the CdSe/CdTe device performance. The nanoscale electrostatic force microscopy (EFM) characterization indicates that the CuSCN layer may be influenced by charge transport on the back surface of CdTe devices due to its wide bandgap. The aqueous NH_4OH based CuSCN provided a smoother surface than that of the DES-based CuSCN layer. With DES as the CuSCN solvent, achieving thin thicknesses of (< 30 nm) is a challenge, using the aqueous NH_4OH as an alternative CuSCN solvent, thinner CuSCN thickness (~ 10 nm) can be acheived in ambient air. The aqueous NH_4OH as the CuSCN solvent reduced the HTL surface roughness preventing the need for high cost DES. By varying the thickness of CuSCN and tailoring the Cu concertation in the CdTe devices, a high PCE was acheived. The solution-processed CuSCNs fabrication used on the CdTe thin-film solar cells could further reduce the cost of solar energy.

#27 Iodine Plasma Erosion of Hollow Cathode Materials

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Current electric propulsion devices have proven their worth for large, conventional satellites. These high-efficiency devices do not meet mission requirements for small, volume constrained spacecraft, though. Trade studies using iodine propellant show superior system-level performance when compared to existing xenon-based systems. As a halogen, iodine introduces a chemical reactivity issue not present in xenon plasmas.

The focus of this research is to develop an iodine plasma material interactivity model at high temperatures for refractory metals typically used in hollow cathodes. Hollow cathodes present unique challenges for use with reactive plasmas because they require conductive materials (metals) to function. These materials are typically more prone to corrosion than ceramics and are operated at extreme temperatures. The duty cycle of electric propulsion requires the cathode operation for long periods of time at temperatures as high as 1700 K.

The experiment has been designed and is currently being demonstrated. The researchers want to prove the approach and make improvements to the process, ensuring accurate, defendable results for the materials of interest. A fundamental aspect of the experiment requires exposure to iodine vapor and iodine plasma separately for similar samples. This approach is expected to quantify erosion rate quantities directly attributed to plasma effects.

#28 Coating Core-shell Cermets for Nuclear Thermal Propulsion Fuel Protection

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New propulsion technologies such as Nuclear Thrust Propulsion (NTP) are being investigated by NASA for space travel. For a material to be viable for NTP technology, it must withstand severe chemical and mechanical conditions (operating temperatures > 2000k and hot hydrogen environment). To test the coating, we use Yittria Stabilized Zirconia as a surrogate fuel material which is coated with Tungsten using unique impeller coating technology (PVD coating). Tungsten is coated at a deposition rate and duration of the coating was varied with each sample to observe the coating morphology and thickness with respect to time. The coating done seemed to peel off and this condition with length of the deposition rate, this could be due to intrinsic stress developed during the coating. To understand the stress development Magnetron sputtering was done on a planar substrate as a function of temperature at constant power of 200W and deposition rate 0.27 nm/s to 0.29 nm/s at constant-pressure of 2 mtorr. The stress seemed to indicate compressive behavior, stress becomes less compressive as temperature increases, and at 300C there appears to be formation of inter-metallic(β-Tungsten) the phase for Tungsten.

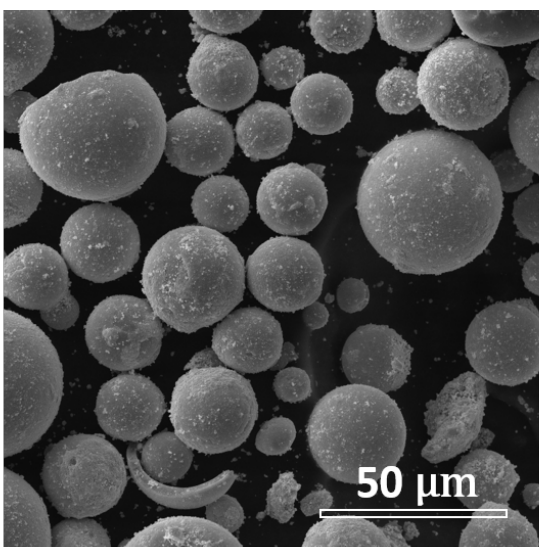

Figure 1 : Morphology of Tungsten coated Yittira Stabilized Zirconia Powders

#29 Influence of Process Parameters on Plasma Surface Modification

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Plasma surface modification has been extensive employed and is of great interest for biomaterials engineering. The influence of various processing parameters affects the degree and rate of surface functionality and has been demonstrated. Herein is described a plasma surface modification of an electrospun biomaterial (polycaprolactone) employing a radio-frequency inductively-coupled plasma (RF ICP) source operating at 13.58 MHz frequency, 45 W power, and 0.8 – 1.0 Torr pressure with ambient atmosphere as process gas introduced at 25 SCCM flow rate. The influence of both time and magnetization of the plasma is demonstrated. The magnetization increases the rate of surface modification with respect to unmagnetized plasma. A cobalt sample introduced into the chamber has an intermediate affect where presumably induced currents will produce a magnetic effect on the plasma modification rate. The influence of process time shows the most significant effects occurring in the early treatment times (< 5 mins) with all processes tending toward equilibrium at longer timescales.

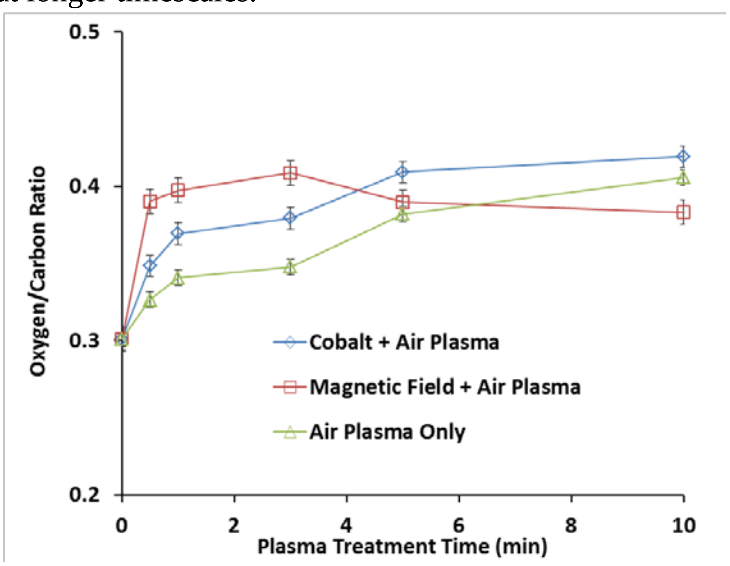

Figure 4. A comparison of the effects of magnetic fields, cobalt metal, in combination with air plasma is shown. The O/C ratios are reported as determined via x-ray photoelectron spectroscopy of the surfaces of the substrate. Error bars are standard deviation for n=3 for each measurement.

#30 Influence of γ-Al_2O_3 addition on oxygen adsorption in CeO_2 nanorods supported Rh catalysts

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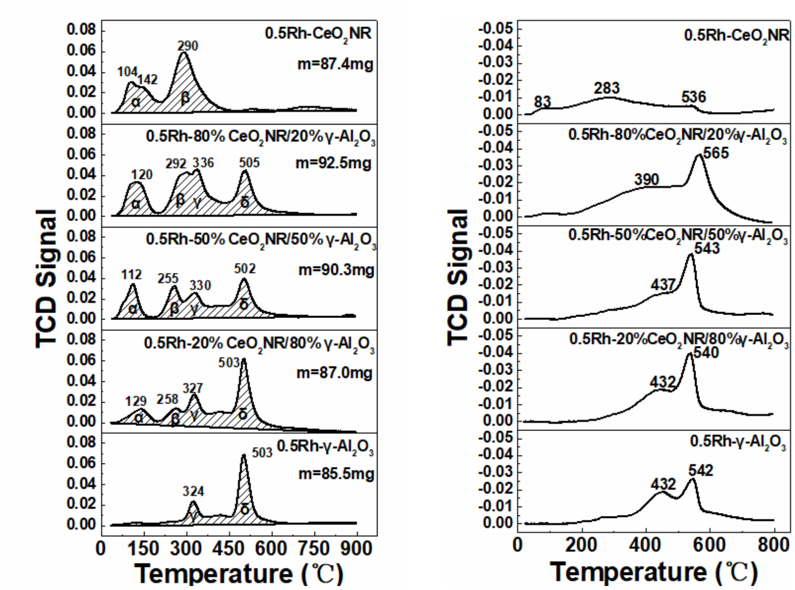
The structural characteristics, adsorption behavior, and catalytic activity of the combination of high-surface-area γ-Al_2O_3 and highly reducible CeO_2 nanorods (NR) supported Rh nanoclusters were investigated. The composite supports with 0%, 20%, 50%, 80%, 100% mole percent of γ-Al_2O_3 were first synthesized using sol-gel and hydrothermal methods, and then 0.5wt% Rh was deposited on each of composites. XRD, Raman spectroscopy, H_2-TPR, O_2-TPD, XPS, TEM and CO conversion were used to characterize these samples without further thermal treatment. Quantitative H_2 consumption on surface and bulk reduction and T_{100} (temperature for 100% CO conversion) of the composites supported Rh catalysts were measured by hydrogen chemisorption and CO oxidation in a fixed bed plug flow reactor system using an online gas chromatograph. The preliminary results indicate that γ-Al_2O_3 addition could enhance the reducibility of CeO_2NR by increasing surface area and low temperature oxygen adsorption, which is critical step for CO oxidation.



A) B)

Figure 1. A) H_2-TPR and B) O_2-TPD of CeO_2NR/γ-Al_2O_3 supported rhodium catalysts.

#31 Au@Pt Nanoparticles on Transparent Electrodes for Spectroelectrochemistry Study of Methanol and Formic Acid Oxidation

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Noble metallic nanoparticles (NPs) such as Au, Ag, and Pt have interesting catalytic and optical properties which plays important role in molecular sensing and alternative energy harvesting, conversion, and storage. Pt layers modified on Au surfaces were recently found to have enhanced electrocatalytic activity for methanol and formic acid oxidation. In this study, Au deposited transparent ITO electrode was further modified by Pt for spectroelectrochemistry study of methanol and formic acid oxidation. The thickness of Pt layer was precisely controlled by deposition cycles. 1, 5, 10, 20, 30 cycles of Pt deposition were performed on Au-ITO to have different Pt coverage. Enhanced catalytic activity was found for both methanol and formic acid oxidation with such structure. The oxidation current density was more than 200 times than that on Au-ITO with Au@Pt(30) sample for both methanol and formic acid. In situ dark field scattering electrochemical study of methanol oxidation in 0.1 M NaOH shows Au NPs were anodized at the potential window of methanol oxidation at lower Pt coverage. Au anodization gets weaker and was terminated with increasing Pt thicknesses. Direct oxidation to CO_2 is favored for formic acid with higher coverage of Pt on Au surface. High-resolution transmission electron microscopy (HRTEM) results confirm the Au-Pt core-shell structure. The present work provides more insights into fuel cell related study on Au-Pt core shell structure.

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POSTER PRESENTATIONS

Material Chemistry

#32 Separating single wall carbon nanotubes：length separation and single chirality isolation

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Separation of single wall carbon nanotubes (SWNTs) are required by assorted applications because of the various length and chirality of pristine material. We used two techniques to separate the single wall carbon nanotubes by length and chirality. The density gradient ultracentrifugation (DGU) was applied for length separation. With an optimized processing procedure, the length distribution was observed from ~600nm to ~60nm by layers, and the yield can be expected up to 1.2ml for each length in one day. A new approach, aqueous two-phase separation (ATPS), was used for isolating the single chirality of SWNTs. We studied the surfactants' influence in a two- phase system, polyethylene glycol (PEG) – dextran solution, for isolating single chirality. We found the concentration of surfactant could control the separation behavior, as the concentration of sodium dodecyl sulfate (SDS) increasing smaller diameter of SWNTs will be partition into PEG phase. The effective SDS concentration was ~0.9wt% to ~ 1.6wt% while kept the DOC concentration under 0.04wt%. The sodium cholate (SC) was added to further separate the metallic- semiconducting SWNTs from the diameter groups of SWNTs.

#33 Oxidation Behavior of Refractory Complex Concentrated Alloys: Computational and Experimental Studies

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High entropy alloys (HEAs) have become a topic of interest due to their compositional complexity and high concentrations of multiple metallic elements. HEAs have been proposed as replacements for conventional materials in an effort to save cost as well as improve properties including oxidation resistance. This work investigates the 1000 °C oxidation performance of a refractory HEA, AlCrHfNbTaTiZr, with regards to the phase distribution in the alloy after annealing at 1100 °C and 1400 °C. Preliminary results on a 5-element alloy, AlHfNbTiZr, which forms a single phase BCC structure was also investigated. The alloy was studied at a range of chemical compositions from equiatomic to lower fractions of Al and Ti while maintaining a single phase microstructure. The phase formation results were compared to thermodynamic simulations runs in ThermoCalc using the CALPHAD method.

#34 Synthesis, characterization and applications of highly modular polyphosphonates

Timothy Ross Totsch, Victoria Stanford*, Ivan Popov**, David French*, and Gary M. Gray**

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Phosphorus-based polymers have exhibited a widespread use in multiple applications such as drug design and delivery, biomedical infrastructure for implants, and as additives in flame-retardants. To further this, our group has expanded this widespread use to the areas of ionic conduction and radioluminescence. Work in this area has led to the successful synthesis of high molecular weight polyphosphonates through a 1:1 molar ratio polycondensation reaction of bis(diethylamino)phenylphosphine ($PhP(NEt_2)_2$) or its anthracenylphosphine derivative ($(C_{14}H_9)P(NEt_2)_2$) with dodecanediol, 1,4-benzenedimethanol and tetraethylene glycol.

The ionic conduction portion of this research was aimed at designing a polyethylene oxide (PEO) backbone to mimic conducting polymers that utilize the ionic interactions with Li^+ to transfer and/or store charge. Materials such as these are desirable for Li^+ ion battery systems but require stability in order to address safety concerns. Phosphorus polymers are widely used for their thermal stability making them candidates conducting materials that are safer than current available options. Additionally, polyphosphonates can be designed using naphthalene or anthracene groups, both of which exhibit X-ray fluorescent properties. The similarity of these polymers to structures such as DNA/RNA make them excellent candidates for biocompatible materials. Thus, these materials may chemically activate Channelrhodopsin-2 (ChR2; a light-gated ion channel) *in vivo*.

#35 The Application of Gibbs Phase Rule and Critical Point Universality to Predict Critical effects in [Title Here, up to 12 Words, on One to Two Lines]

Xingjian Wang[$, %](xw0006@uah.edu)

Advisor: James K. Baird[$, %, &] (bairdj@uah.edu)

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Abstract

According to the Griffiths and Wheeler postulate, the critical effect exists in the system when one density variable is held fixed. We have predicted the existence of critical effects on the solubility of solid-liquid equilibria in binary liquid mixture with a critical point of solution by the Gibbs phase rule analysis. The critical point universality also predicts the same critical effects in both physical and chemical solid-liquid phase equilibria. Those predictions are proved by the results of three experiments including: (1) dissolution of phenolphthalein in the nitrobenzene and dodecane (physical solid-liquid phase equilibria); (2) dissolution of barium chromate in the isobutyric acid (IBA) + water (chemical solid-liquid phase equilibria); (3) dissolution of lead sulfate and lead iodide in the IBA + water(chemical solid-liquid phase equilibria). When the concentration of solute is plotted in van't Hoff form, the slop diverges toward negative infinity for the endothermic reaction is endothermic and toward positive infinity for the exothermic reaction. From the data of barium chromate experiment, we also use the spline fit method to determine the critical exponent of solubility equals β.

POSTER PRESENTATIONS

Bio/organic materials

#36 3-Dimensional Bio-printing of Composite GelMA/PCL Scaffolds

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Now in recent days 3d printing has become an important tool in all fields specially in the field of medical it allows you freedom to manufacture artificial body parts still it's in initial stage researchers are working on printing of actual human body organs. For that cell growth outside the body is main parameter. This study is mainly focused on developing the scaffolds with various polymers crosslinking with materials which helps for cell growth. PCL is used as a polymer in this study as a main scaffold material. Various types of scaffolds with change in design were printed with the help of printer which build for printing of biomaterials. Scaffolds with various design, different pore sizes were printed which then crosslinked with Gelma to analyze their characteristics. Some scaffolds were plasma treated to study its effect on the mechanical and thermal properties of material. Thermal characteristic analysis like DSC, FTIR, TGA was also performed on the scaffolds. This poster will give idea about the effect of design, crosslinking material on the scaffolds.

#37 Rapid Diagnostics of Mycobacteria with Lectin Conjugated Silica Coated Magnetic Nanoparticles

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Development of a fast, rapid and sensitive bacterial determination method is crucial in medical diagnostics. Tuberculosis is caused by bacteria *Mycobacteria tuberculosis* (Mtb) is a highly contagious illness causing approximately one million deaths per year. Current methods of Mtb detection are time-consuming, labor intensive and expensive. We have developed a rapid diagnostic method of detecting Mycobacteria using lectin conjugated silica coated magnetic nanoparticles (SMNPs). The lectin Concanavalin A (ConA) and Aleuria Aurantia Lectin (AAL) recognize the mannose and arabinose carbohydrate epitopes found in the cell wall of the Mycobacteria. The multivalent Con A/AAL conjugated SMNPs bind to the bacterial cell wall and crosslink the bacteria within minutes to form a visible precipitate without the need of any instrumentation. Control studies were done with orally abundant cross contaminating microorganisms such as *Streptococcus mutans* and other non-binding proteins such as Wisteria Floribunda Lectin (WFL) and Bovine Serum Albumin (BSA). SMNPs conjugated with Mtb polyclonal antibodies are used to compare the binding efficiency of Con A and AAL conjugated SMNPs.

#38 Functionalized Hollow Mesoporous Silica Nanoparticles as an Efficient Carrier of Antibiotics

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An efficient antibiotic delivery platform is designed using hollow mesoporous silica nanoparticles (HMSNs) to target and deliver a cargo of antibiotics to gram-negative Mycobacteria. HMSNs are synthesized by co-condensation of 3-aminopropyltriethyoxy silane and tetraethylortho silicate in the presence of ammonia and cetyltrimethylammonium bromide (CTAB) as pore forming agent. The large hollow interior of nanoparticles is used as a reservoir for small molecule antibiotics. We use these well-defined mesoporous channels to diffuse antibiotics like colistin and isoniazid to the exterior microenvironment of the bacteria cell increasing the local concentration of antibiotics. Active targeting of Mycobacteria is achieved via a plant lectin Aleuria Aurantia (AAL). AAL is conjugated to the surface of HMSNs (AAL-HMSNs). AAL binds to Mycobacteria cell surface carbohydrate - arabinose. Colistin (col), a cationic antimicrobial peptide is electrostatically attracted to the interior and exterior surface of HMSNs via phosphonate silane (Col-AAL-HMSN). Small molecule isoniazid (INH) is conjugated to the surface using a heterobifunctional linker perfluorophenylazide silane (INH-AAL-HMSN). We observed that using that several folds lower amount of antibiotics is necessary to reach minimum inhibitory concentration when associated with HMSNs compared to free antibiotics.

#39 Investigation of the crystallinity index (CI) and crystallite sizes of four bamboo species using X-ray diffraction (XRD) technique

Bahrum Prang Rocky[1] and Amanda J. Thompson[2]

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The presence of crystallinity in polymers determines properties, such as strength, elasticity, toughness, brittleness, stiffness, rigidity, chemical resistance, melting temperature, density, optical and dyeing properties. The degree of crystallinity or crystallinity index (CI) of cellulose-based plants can be an indicator whether the material has potential for fiber application. This study was conducted on four bamboo species: red margin, moso, giant gray and bissetii to determine the CI and crystallite sizes using x-ray (Cobalt source) diffraction (XRD) that is newly applied but the most direct technique to assess fiber. By separating crystalline and amorphous phases from the diffracted graph, the CI of the four bamboo plants were determined by using two methods: 1) from the height of the crystalline and amorphous peaks, and 2) from the area under crystalline and amorphous regions. The CIs were found to be 59.60%, 63.06%, 62.81% and 65.68% from method 1, and 58.58%, 63.04%, 62.77% and 64.34% from method 2 respectively. The crystallite sizes were 36.79, 36.04, 36.83 and 36.40 Å of four species respectively. The peaks were identified on $101, 10\bar{1}$ and 002 reflection planes at ~18.5°, 19.8° and 25.5° Bragg's angles. The techniques were consistent and suitable in multiple tests to estimate the results.

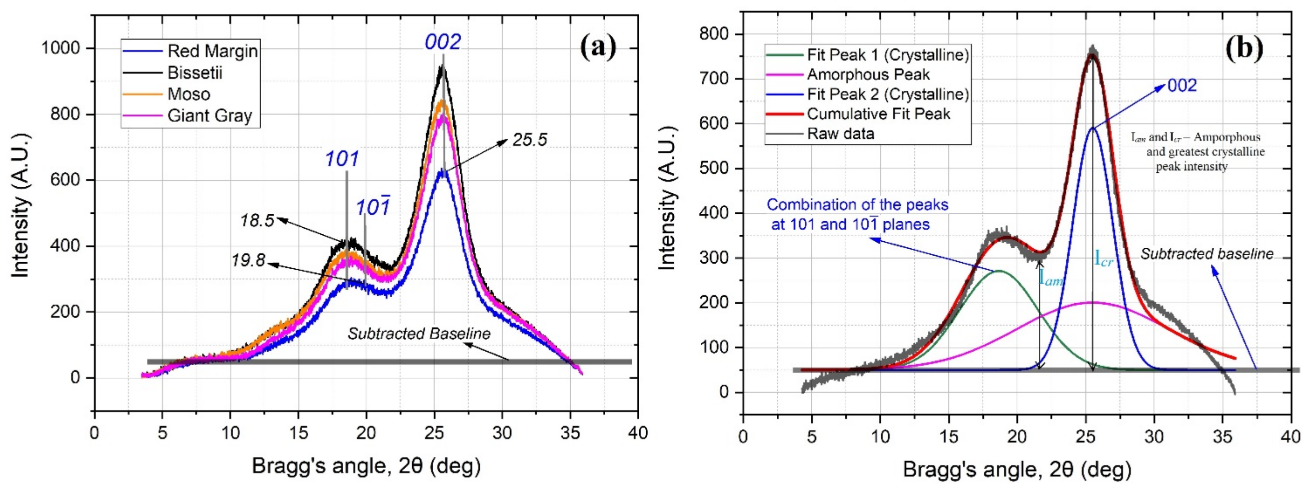

Figure 1. X-ray diffraction (a) peaks of four bamboo species to determine crystallinity index and crystal sizes, and (b) FitPeak processing using *Origin Pro* on Moso bamboo XRD data.

POSTER PRESENTATIONS

Nanomaterials

#40 Growth and Electrical, Nano-Optical Characterization of semiconducting MoS_2/WS_2 in-plane Heterostructures

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In-plane heterojunctions of atomic-thick (2D) semiconductors (MoS_2/WS_2) are novel structures that can potentially pave the way for efficient ultrathin and flexible optoelectronics, such as light sources and photovoltaics. Such heterostructures (HS) are very rare and not much is known about their characteristics. They can only be achieved through a synthetic growth process such as chemical vapor deposition (CVD). This is unlike vertical heterostructures, for which the materials can be mechanically stacked one layer on top of the other. The CVD growth of in-plane heterostructure is a thermodynamically driven process and presents a number of challenges to control the vapor pressure of the precursors. Additionally, new analytical tools need to be developed in order to gain access to and understand the physical properties of these HS.

Here, we report a one-step CVD growth of monolayer (1 nm) thick MoS_2/WS_2 in-plane heterostructures. We have characterized their morphological and optical properties using micro-Raman and photoluminescence spectroscopy. Kelvin probe force microscope was used to extract the surface potential profile across the MoS_2/WS_2 heterojunction boundary, which was then used to gain access to fundamental semiconductor heterostructure parameters such as depletion layer width and built-in field across the MoS_2-WS_2 interface.

#41 Pinning Strength Quantification of Solute Concentrations at Specific Grain Boundaries.

Authors: David Jacobson[1,2], Stephen Foiles[2], Fadi Abdeljawad[2], Gregory B. Thompson[1]

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A computational method has been developed to calculate the pressure required for grain boundaries to overcome the pinning effects of second phase particles. Multiple Pt bicrystals were constructed with small concentrations (<= 0.5 atom %) of Au segregated to the boundary using the Monte Carlo method. Molecular dynamics simulations employing the artificial driving force method were carried out on said boundaries to measure the relationship between boundary type, solute concentration, and boundary velocity. It was found that for a given solute concentration there exists a critical driving pressure necessary for grain boundary motion to occur. Sub-critical driving pressures resulted in flexing of the grain boundary about the pinning precipitates, but with no large scale grain boundary movement. Above critical driving pressures resulted in grain boundary motion although the amount of time required for grain boundaries to break loose from the pinning structures varied considerably. At solute concentrations of 0.1%, solute segregation to the boundary did not occur. The resulting lack of precipitates caused boundaries to behave no differently from pure boundaries, although at real timescales a reduction in mobility would be exhibited because of solute drag.

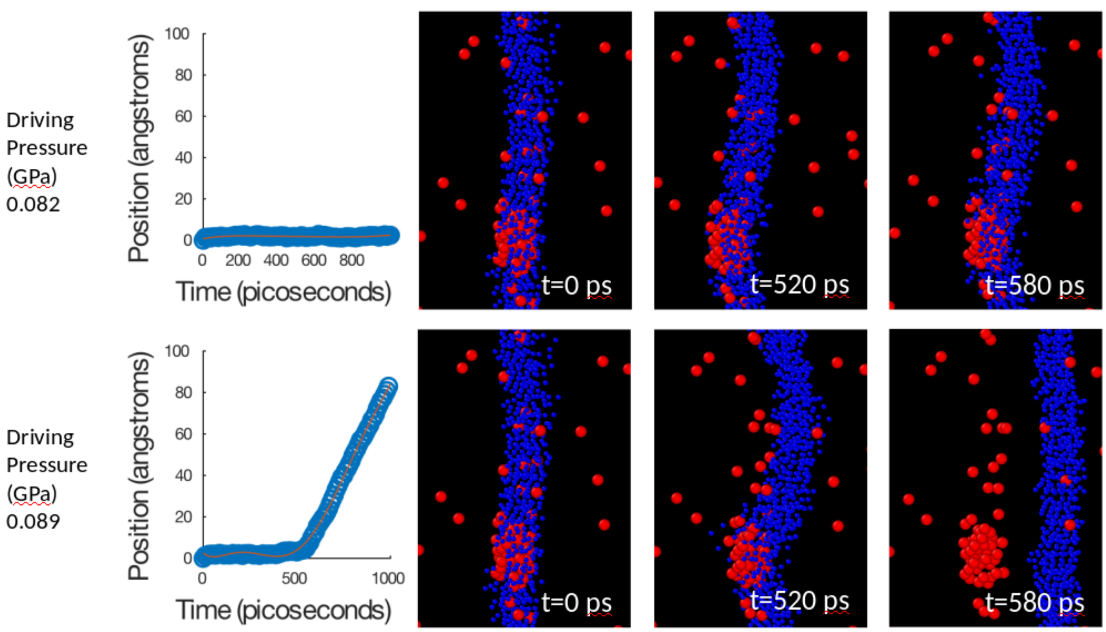

Figure 1: Simulation rendering of grain boundary breakaway from precipitates with associated graphs showing the change of the grain boundary position with time.

#42 Comparison of electrical properties of PLZT thin film capacitors using coplanar and interplanar electrode configuration

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In this work, metal/ferroelectric/metal (MFM) capacitors were fabricated using ferroelectric thin films of $Pb_{0.95}La_{0.05}Zr_{0.54}Ti_{0.46}O_3$ (PLZT). Films were prepared using chemical solution deposition method and metal electrodes were vacuum deposited using a shadow mask. Capacitors with two electrode configurations viz. coplanar (Au/PLZT/Au) and interplanar (Au/PLZT/Pt) used to measure electrical properties showed different electrical behavior. For coplanar configuration, higher polarization and coercive voltage were obtained under illumination as compared to interplanar electrode configuration. Further, the capacitors with coplanar configuration also demonstrated higher PV parameters, such as short circuit current density (J_{sc}) and open circuit voltage (V_{oc}). As an example, J_{sc} of 1.86 µA/cm^2 and V_{oc} of -1.1 V were obtained using coplanar configuration with Au electrodes for unpoled devices. Poling showed an improvement in PV parameters for both the coplanar and interplanar configurations, with higher values obtained from the coplanar configuration. After poling, J_{sc} of 1.32 µA/cm^2 and V_{oc} of -0.93 V for interplanar configuration, and J_{sc} of 2.04 µA/cm^2 and V_{oc} of -2.01 V for coplanar configuration were obtained. These results suggest that coplanar configuration is better for measuring the photovoltaic properties of PLZT thin film based capacitor structures. Thus, the selection of electrode configuration is essential for designing ferroelectric photovoltaic devices.

#43 Thermomechanical Testing of Free-Standing Thin Films: A Novel Experimental Technique

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A novel technique for thermomechanically deforming thin films has been developed to investigate the fundamental mechanisms governing deformation of such 2D materials at elevated temperatures. Specimens fabricated through the combination of spin-coating photoresist and DC sputter deposition through machined shadow masks were subjected to an acetone bath to liberate free-standing thin films. The photoresist acted as a sacrificial layer, allowing the films to be deposited as near-atomically smooth structures while providing enough support for the films to be transferred to test grips. Mechanical loading was conducted through a commercial in-situ scanning electron microscope tensile testing unit in an inert environment; optics-driven heating provided the ability to uniformly heat specimens to temperatures greater than half their melting temperature, as measured by a pyrometer, while load was applied. The stress-strain relationship in nanocrystalline Ni thin films has been investigated at room temperature through the same tensile testing apparatus which provides preliminary results for reference.

#44 Literature Review of the effects of DC Bias in the nucleation of BN thin films in Chemical Vapor Deposition (CVD)

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Boron Carbon Nitride (B-C-N) ternary, and other high Boron content thin films can be synthesized by CVD onto Silicon substrates. Applying a DC-Bias to the substrate can result in energetic projectiles in the form of ions that bombard near-surface atoms. Experiments have shown that such ion bombardment is essential for the formation of the cubic phase of boron nitride; without it, only sp^2 BN thin films can be produced. Computer simulations have shown how ion bombardment can make sp^2 BN transition into sp^3 BN at the atomic level. Using literature from previous experiments synthesizing cubic-Boron Nitride (cBN), we consider designing future experiments using CVD to synthesize boron-rich thin films, several compounds of which are expected to be superhard. This poster reviews and summarizes previous literature on the theoretical and experimental investigations of ion bombardment for the synthesis of cBN thin films. The physical and chemical properties at the atomic scale will be described. We have access to microwave plasma Chemical Vapor Deposition (CVD), in which diborane, ammonia, and methane gas can be used to synthesize B-C-N and other Boron-rich thin films.

#45 Using ImageJ to analyze SEM micrographs of Nano/microscale fibers

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Analyzing images such as SEM and TEM micrographs is a very important process for the characterization of fibers. In past, researchers needed measure the length and diameter of fibers by hand; and, this is cumbersome and error-prone. Fortunately, National Institute of Health (NIH) has developed Image J to solve this question. Image J is a professional and convenient software which can edit and analyze various image file formats, including GIF, TIFF, PNG, JPEG, FITS, etc. In our research, we use Diameter J plug-in to measure the diameter of fibers correctly and rapidly through the SEM images. Firstly, we convert an image into a binary representation by segment fibers and background. Then, we set the length unit. Finally, we use Diameter J to analyze the image automatically and obtain the output.

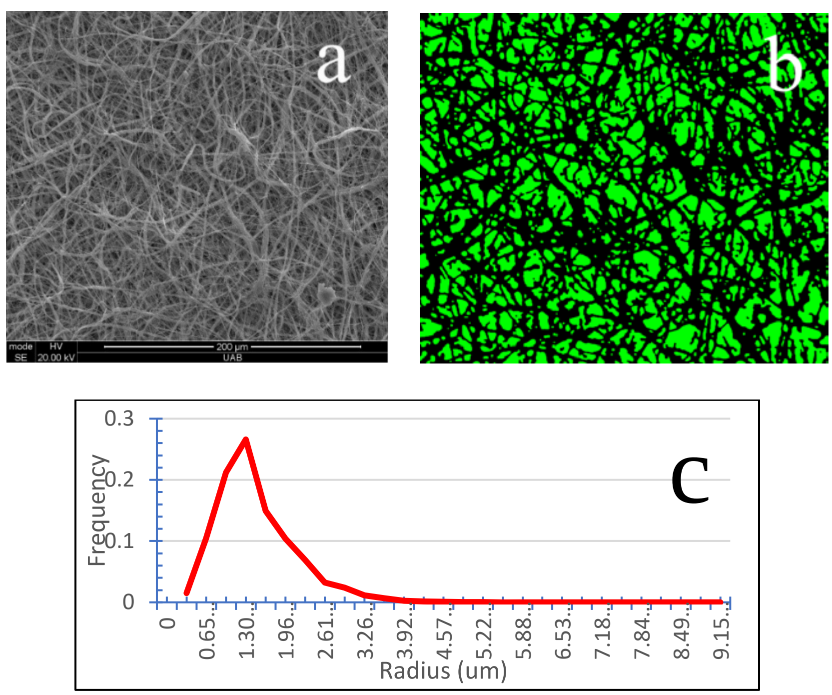

Figure 1. The analyze process; (a) Original SEM image; (b) Binary representation by segment fibers and background; (c) The radius distribution

#46 Substrate Deformation from Aerosol Deposition of Barium Hexaferrite Film

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Abstract

Barium Hexaferrite (BaM) films grown on sapphire substrate by aerosol deposition have been investigated to determine the nature of energetic damages inherent in the growth method. Energy dispersive x-ray spectroscopy (EDS) mapping reveals Al_2O_3 particulates throughout the BaM film, likely ejected from the substrate surface during growth. The concentration of Al_2O_3 particles is higher at the substrate-film interface but persists throughout the 6 µm film. X-ray diffractometry analysis shows an increase in polycrystalline Al_2O_3 peak intensity up to 1.2 µm from the film-substrate interface and subsequent decrease at higher thicknesses, suggesting a population of randomly-oriented Al_2O_3 particulates that decreases in density further from the substrate. Alternating gradient magnetometry shows a significant drop in magnetic moment density as a function of thickness consistent with the replacement of BaM with Al_2O_3 in the volume fraction estimated by EDS mapping. At high thicknesses, we find that the BaM film suffers a slight drop in the magnetic moment with respect to the volume fraction model, likely explained by x-ray absorption spectroscopy measurements showing a small but measurable amount of Fe reduction from Fe^{3+} to Fe^{2+}.