2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Keynote Session on Nanomaterials, General Properties and Others

Sponsored by: TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Monday 8:30 AM
February 17, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Haiyan Wang, Texas A&M University; Ravindra Nuggehalli , NJIT

8:30 AM Keynote

Frontiers in Thin Film Epitaxy and Novel Nanostructured Materials: *Jagdish (Jay) Narayan*[1]; [1]North Carolina State University

This talk focuses on designing and processing of novel nanostructured materials of controlled size and orientation, and defects and interfaces (1). Thin film growth modes can be precisely controlled to produces zero- one-, two-, and three-dimensional nanostructures. The orientation control requires epitaxy across the misfit scale which is achieved by the paradigm of domain matching epitaxy. The DME paradigm emphasizes the matching integral multiples of lattice planes across the film-substrate interface, where domains are separated by dislocations and the misfit inbetween the integral multiples is accommodated by the principle of domain variation. This talk emphasizes on two-dimensional psuedomorphic metamaterials where the chemical composition is controlled by growth parameters and the structure is determined by the structure of the substrate which provides a template for thin film growth. The thickness (1-5 monolayers) can be controlled manipulating strain and internal thermodynamic free energy. (1) J. Narayan, “Recent progress in thin film epitaxy across the misfit scale,” Acta Materialia 61, 2703-2724 (2013).

9:10 AM Keynote

Probing Structure, Properties and Dynamics of Nanostructures through Scanning Transmission Electron Microscopy: *Stephen Pennycook*[1]; Wu Zhou[1]; Jaekwang Lee[1]; Juan-Carlos Idrobo[1]; Myron Kapetanakis[2]; Junhao Lin[2]; Sokrates Pantelides[2]; [1]Oak Ridge National Laboratory; [2]Vanderdbilt University

The aberration-corrected scanning transmission electron microscope (STEM) now allows direct, real space imaging at atomic resolution and low accelerating voltages to minimize damage. In two-dimensional materials such as BN and graphene, atom-by-atom characterization of atomic position, atomic species, chemical bonding and optical and electronic properties is feasible. Furthermore, through direct momentum transfer, the STEM probe can also reveal the dynamics of small clusters, which can be compared to density functional calculations to determine the energy landscape. Examples will be shown of a Si6 cluster in a graphene nanopore and metallic transition metal chalcogenide nanowires which self assemble with ohmic contacts to the surrounding two-dimensional layers. Research supported by DOE BES Materials Sciences and Engineering Division (SJP, JL, STP), ORNL’s ShaRE User Program, sponsored by DOE-BES (J-CI), an ORNL Wigner Fellowship (WZ), NSF DMR-0938330 (WZ, J-CI), DOE grant DE-FG02-09ER46554 (MK, JL, STP) and the McMinn Endowment (STP) at Vanderbilt University.

9:30 AM Keynote

Design and Applications of Nanostructured Energy Materials: *Sungho Jin*[1]; [1]UC San Diego

There is a strong need for advanced energy materials for harvesting of green energy. Energy materials having controlled nanoscale configurations offer a promise of much improved efficiency. In dye sensitized solar cells, photoanode nanostructures incorporating elongated nano conductors can provide a significant enhancement in the energy conversion performance and reliability. For water splitting hydrogen generation, a very large surface area electrode decorated with a uniform distribution of nanosized photocatalyst particles is desirable. For thermoelectric materials, the formation of nanograined alloy structure with a modulation doped layer is useful for optimizing the thermal conductivity and achieve increased figure of merit. For photovoltaic solar cells and solar thermal devices, nanoscale surface structures are desirable for enhanced light absorption and high performance energy conversion. In this presentation, various means for creating and controlling nanostructures in different types of energy materials will be described, and their implications for technical applications will be discussed.

9:50 AM Keynote

Nanogenerators for Self-powered Systems and as Active Sensors: *Zhong Wang*[1]; [1]Georgia Institute of Technology

We demonstrate a simple, low cost and effective approach of using the charging process in friction to convert mechanical energy into electric power for driving small electronics. The triboelectric nanogenerator (TENG) is fabricated by stacking two polymer sheets made of materials having distinctly different triboelectric characteristics, with metal films deposited on the top and bottom of the assembled structure. Once subjected to mechanical deformation, a friction between the two films, owing to the nano-scale surface roughness, generates equal amount but opposite signs of charges at two sides, respectively. Thus, a triboelectric potential layer is formed at the interface region if the generated triboelectric charges are separated by a small distance; the electrons in the external load are driven to flow for generating an induced potential for screening the triboelectric potential. This is the mechanism of the trioboelectric nanogenerator.

10:10 AM Break

10:30 AM Keynote

Magnetoelectric Control of Exchange Coupling in Monodomain BiFeO3 Heterostructures : *Chang-Beom Eom*[1]; [1]University of Wisconsin-Madison

Multiferroic materials that exhibit coupling of ferroelectric and antiferromagnetic ordering form the basis of exciting heterostructures that can provide electric field control of magnetization. Such structures provide new directions for novel spintronic devices. In particular, the electric field control of exchange bias coupling to a ferromagnetic layer forming one electrode of a magnetic tunnel junction provides unprecedented control. Here we investigate the exchange coupling between monodomain multiferroic BiFeO3 (BFO) and a soft ferromagnetic Co overlayer. We use x-ray magnetic circular dichroism (XMCD) and anisotropic magnetoresistance (AMR) to investigate these heterostructres. We demonstrate that the exchange coupling between BFO and Co occurs without the contribution of domain walls. device applications.This work has been done in collaboration with W. Saenrang, B. A. Davidson, S. Ryu, J. Podkaminer, D. Lee, J. Frederick, T. Kim, S. Baek, M.S. Rzchowski, J. Freeland.

10:50 AM Keynote

Stress-engineered Self-organized Nanostructure Array Assembly: A Rich Paradigm: *Anupam Madhukar*[1]; [1]University of Southern California

Two- and three-dimensional regular arrays of quantum confined nanostructures such as quantum wires and quantum dots constitute a basic and powerful platform for realization of electronic and optoelectronic technologies that underlie information sensing and processing systems for applications ranging from communications to energy conversion and biomedicine. The most successful growth-controlled approach to realizing such architectures to-date exploits engineering surface stress gradients to manipulate atomic migration direction and molecular reactions during growth and growth interruption. In this talk I will address the current status of the subject through illustrative examples of both lattice-matched and mismatched semiconductor combinations focusing on (a) the significance of the kinetics of atomistic processes in controlling the assembly and nature of the resulting quantum nanostructures, and (b) some key issues that require much deeper understanding to enable realizing the full potential of this powerful approach.

11:10 AM Keynote

Mechanical Behaviors of Heterogeneous Nanostructured Metals: *K. Lu*[1]; [1]Chinese Academy of Sciences

In comparison with the strong-but-brittle homogeneous nano-grained metals, heterogeneous or hierarchical nanostructured metals are found to exhibit promising property combinations, such as simultaneous increment of strength and fracture toughness, and of strength and tensile ductility. In this talk, mechanical behaviors of three types of heterogeneous nanostructured metals will be introduced: (i) ultrafine-grains with nano-scale twins, (ii) nano-twinned grains mixed with coarse grains, and (iii) gradient nano-grained (GNG) structures. Mechanical properties including strength, ductility, work-hardening, rate sensitivity, and fatigue behaviors will be discussed with respect to the heterogeneous nanostructures with emphases on the nano-scale size effects. Several examples will be presented for illustrating the correlation between these heterogeneous nanostructures and their mechanical behaviors. Perspectives on heterogeneous nanostructured metals will be addressed as well.

11:30 AM Keynote

The Principles of Grain Refinement during Severe Plastic Deformation: *Terence Langdon*[1]; [1]Univ of Southern California

The application of severe plastic deformation (SPD) to bulk materials provides an opportunity for achieving exceptional grain refinement to the submicrometer or even the nanometer level. Several SPD processing methods are now available but the most attractive are equal-channel angular pressing (ECAP) and high-pressure torsion (HPT). This presentation examines the principles of grain refinement in these two processing methods with emphasis on the magnitudes of the final grain sizes.

11:50 AM Keynote

Influence of Length Scales on Precipitation Phenomena in Al Alloys: Tao Hu[1]; Julie Schoenung[1]; *Enrique Lavernia*[1]; [1]University of California, Davis

Nanostructured metals and alloys have engendered scientific and technological interest, partly due to the discovery of novel deformation mechanisms, which provide a pathway for enhanced mechanical behavior. Much of the original research was conducted using pure metals and binary alloys systems. Recently, however, research has evolved to encompass precipitation-strengthened systems due to the fundamental questions related to the precipitation phenomena in nanostructured alloys that require investigation and the potential for increased mechanical performance via precipitation strengthening. In this lecture we will discuss recent results related to the influence of length scales on precipitation phenomena in Al alloys. Precipitation phenomena will be described in terms of the type, morphology, size and distribution of precipitates as a function of different length scales. In addition, the influence of defects, e.g. dislocations and grain boundaries, on the nucleation and growth of the precipitates at different length scales in precipitation-hardened Al alloys is also addressed.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Keynote Session on Nanomaterials and Applications
Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Monday 2:00 PM
February 17, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Ke Lu, Institute of Metal Research; Dieter Wolf, Argonne National Laboratory

---

2:00 PM Keynote
Colossal Injection of Catalyst Atoms into Epitaxial Silicon Nanowires: *David Seidman*[1]; Oussama Moutanabbir[2]; Dieter Isheim[1]; Horst Blumtritt[3]; Stephan Senz[3]; Eckhard Pippel[3]; [1]Northwestern University; [2]Ecole Polytechnique de Montreal; [3]1Max Planck Institute of Microstructure Physics
The incorporation of impurities during growth of nanowires from the vapour phase alters deeply their basic properties with impacts on an extended range of emerging nanoscale technologies. Herein, we present an atomistic level and quantitative study of the phenomenon of catalyst dissolution by achieving three-dimensional atom-by-atom maps of individual aluminium catalyzed silicon nanowires using highly focused ultraviolet laser-assisted atom-probe tomography. Although the observed incorporation of the catalyst atoms into nanowires exceeds by orders of magnitudes the equilibrium solid-solubility and solid-solution concentrations in known non-equilibrium processes, aluminium impurities are homogeneously distributed and do not form precipitates or clusters. Besides inducing p-type doping, this kinetics-driven colossal injection also has direct implications for nanowire morphology. The current theories of solute trapping at moving interfaces cannot explain the observed phenomenon. Herein, a rate equation model is presented to describe catalyst atoms incorporation during step-flow growth of a silicon nanowire.

2:20 PM Keynote
Solidification Mechanisms of Carbon as Graphene, Graphite and Diamond from Metal-carbon Melts: *Reza Abbaschian*[1]; Shaahin Amini[1]; [1]University of California, Riverside
The formation of three allotropes of carbon as graphene, graphite and diamond from supersaturated metal-carbon melts will be reviewed. For the formation of graphene, it is shown that a single sheet of carbon atoms with a honeycomb lattice nucleates and grows on the melt surface upon cooling. Beside the nano-crystalline layer, bulky flaky or spherical graphite may also form in the interior of the melt. Small solidification rates favor formation of flake graphite because of the limited 2-dimensional nucleation and spreading along basal facets. At higher rates, on the other hand, both basal and prismatic faces grow with a similar rate, leading to the spherical morphology. When the melt is exposed to exceeding pressures of 5.0 – 6.5 GPa, carbon crystallizes as diamond. The diamond crystal morphology and quality also strongly depend on the growth temperature and atomistic growth processes taking place at the diamond–molten metal interface.

2:40 PM Keynote
Fundamentals of Ion-solid Interactions in Ceramic and Structural Materials: *Steven Zinkle*[1]; [1]Oak Ridge National Laboratory
Ion bombardment can create a wide variety of novel nanostructures and nanoscale chemical profiles in materials, with resulting unique materials properties. The field of ion-solid interactions is one of numerous topics that have richly benefitted from the research by Jay Narayan. This presentation will summarize some of the defect architectures that can be created in ion-bombarded materials, including defect cluster patterning (cavities and dislocation loops) and solute precipitation (e.g., metallic colloid formation in insulators). The impact of these nanostructures on materials

properties will be discussed and related to fundamental aspects of ion-solid interactions including the roles of irradiation temperature, damage rate, and primary knock-on atom spectra. Unresolved scientific issues including the role of ionization on point defect diffusion in nonmetals and the potential impact of one-dimensional glissile transport versus three-dimensional random walk diffusion of point defect clusters will be highlighted.

3:00 PM Keynote

Hierarchical Microstructural Architecture for High-performance Thermoelectrics: *Vinayak Dravid*[1];
[1]Northwestern University

The intellectual challenge for the next generation bulk thermoelectric materials revolves around synthesis and fabrication of hierarchically organized microstructure that does not appreciably compromise the innate high power factor of the chosen thermoelectric matrix systems but significantly reduces lattice thermal conductivity to enhance the overall figure of merit, ZT. An emerging strategy involves nanostructuring bulk thermoelectric materials; wherein nanoscale precipitates do not appreciably compromise charge transport (thus power factor) but significantly reduce the lattice thermal conductivity via phonon scattering pathways. Here, there are exciting opportunities for understanding and tailoring microstructural elements with attention to the hierarchical length-scale influence from atomic-, nano- and micro-meter dimensions. We demonstrate this intricate but tractable relationship between various microstructural attributes (atomic-scale, line and interfacial defects as well as associated elastic and plastic strain) and lattice thermal conductivity. The presentation will also cover strategies for next generation thermoelectrics based on hierarchical length-scale tailoring of microstructure.

3:20 PM Break

3:40 PM Keynote

Coarsening of Nanoscale Precipitates in Al-Li Alloys: *Martin Glicksman*[1]; Ke-gang Wang[1]; Ben Pletcher[2];
[1]Florida Institute of Technology; [2]Select Arc Corp.

Precipitates nucleate in dilute Al-Li alloys as a distribution of spherical nanoscale particles with diameters <10 nm. Analysis of their dynamic evolution via diffusion-limited coarsening allows quantitative evaluation of collective interactions called ‘diffusion screening’. Debye-Huckel theory and multiparticle simulations serve as predictive methods for interpreting late-stage coarsening kinetics in these precipitation-hardened alloys. Particle size distributions, growth kinetics, and maximum-allowed particle sizes were measured with automated TEM and HREM, and compared with theoretical and computational predictions. The dependence of the rate constants on precipitate volume fraction and their associated dynamically admissible size ranges were evaluated for the first time. Our experiments show that diffusion screening, a fundamental interaction among fine-scale dispersions, yields reasonable kinetic predictions of the observed d' (Al3Li) dispersions. Multiparticle simulations of precipitate evolution are compared with experiments. Diffusion screening theory and simulation models provide useful tools for the future design of two-phase alloys for elevated temperature applications.

4:00 PM Keynote

Plastic Deformation in Nanoindentation of a BCC Metal: *Marc Meyers*[1]; Carlos Ruestes[1]; Tane Remington[1]; Eduardo Bringa[2]; Bruce Remington[3]; Bimal Kad[1]; [1]UCSD; [2]CONICET/U. Nacional de Cuyo; [3]LLNL

Experiments and molecular dynamics calculations reveal the mechanisms of deformation under a nanoindentation in tantalum, chosen as a model BCC metal. Both molecular dynamics calculations and indentations are conducted for three monocrystal orientations: [100], [110], and [111]. The evolution of plastic deformation proceeds by the initiation through nanotwins and stacking faults, which evolve to shear dislocation loops. They expand into the material by the advance of the edge component. Simultaneously with this advance, the screw components of the loop cross slip and describe a cylindrical surface. When the opposite segments approach they attract each other and eventually cancel, forming a quasi-circular prismatic loop in the process composed of edge dislocation segments. The prismatic loops advance into the material along the <111> directions. Analytical calculations supplement the molecular dtynamics and experimental observations and provide a framework for the improved understanding of the evolution of plastic deformation under a nanoindenter.

4:20 PM Keynote

Strengthening of Steels by Nanodispersoids: *G Sundararajan*[1]; R Vijay[1]; [1]ARCI

The strengthening of steels by micrometer sized dispersoids is well understood. However, only in the last decade, it has been possible to produce steels containing a high number density of nanometer sized dispersoids. These steels, normally designated as oxide dispersion strengthened (ODS) steels, display outstanding high temperature mechanical behaviour and in addition exhibit excellent fatigue and irradiation resistance. The objective of the presentation is to examine the evolution of nano dispersoids in Fe, Fe-9Cr and Fe-18Cr steels in terms of their structure and size, right through the processing steps, starting from atomisation, followed by milling and consolidation and finally by hot extrusion and subsequent annealing. The influence of nano dispersoids on the elevated temperature properties of the steels will be evaluated in terms of the applicable strengthening mechanisms. In addition, the reasons behind the substantial decrease in the yield strength beyond 600 deg C will be discussed.

4:40 PM Keynote

Role of Dislocations during Processing and Deformation of Nanocrystalline Materials: *Farghalli Mohamed*[1]; [1]University of California,Irvine

Nanocrystalline (nc) materials, which are characterized by grain sizes = 150 nm, offer interesting possibilities related to many structural applications. Therefore, it is no surprise that considerable efforts have been devoted to investigating nc-materials over the past two decades. These efforts have resulted in major advances. Primary among these advances is the identification of the role that dislocations play not only in processing nc-materials via severe plastic deformation (SPD) but also in accounting for their mechanical behavior. Details of this role will be presented.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Poster Session

Sponsored by: TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Monday 6:30 PM
February 17, 2014
Room: Sails Pavilion
Location: San Diego Convention Center

Session Chair: Sudhakar Nori, North Carolina State University; Ravindra Nuggehalli, New Jersey Institute of Technology

---

Effect of Growth Parameters on Electrical and Optical Properties of Ga and Al Doped Transparent Conducting Zinc Oxide Thin Films: Structure-property Correlations: *Namik Temizer*[1]; Sudhakar Nori[1]; Jagdish Narayan[1]; [1]North Carolina State University

The optoelectronic properties of ZnO thin films depend highly on the deposition and growth conditions as these properties change significantly with the dopant, the oxygen flux during film deposition and substrate temperature. Here, we present a systematic study of the structure-property correlations in Ga and Al doped ZnO thin films on c-sapphire where the microstructure varies from nano-crystalline to single crystal films. We have achieved films with lowest resistivity (~110 µO-cm) and highest optical transmittance (~90%) characteristics. The films grown at $5x10^{-2}$ Torr of ambient P_{O_2} and at growth temperatures ranging from room temperature to $600^{o}C$ show semiconducting behavior, whereas films grown at P_{O_2} of $1x10^{-3}$ Torr show metallic behavior. The most striking feature is that the resistivity minima occur at high temperatures ~75K. We propose that formation of Oxygen vacancy-Zinc interstitial defect complex (V_O-I_{Zn}) is responsible for the significant concurrent enhancements in n-type conductivity and optical transparency.

Fabrication of Single crystalline NiO based P-N junctions by KrF Laser Treatment: Structure and Photochemical Properties.: *Roya Molaei*[1]; M.Reza Bayati[1]; Jay Narayan[1]; [1]NC State University

We report the formation of NiO based single crystalline p-n junctions with enhanced photocatalytic activity induced by pulsed laser irradiation. The NiO epilayers were grown on Si(001) substrates buffered with cubic yttria-stabilized zirconia (c-YSZ) by using pulsed laser deposition. Microstructural studies conducted by X-ray diffraction (?-2? and f techniques) and high resolution TEM. The p-type electrical characteristics of the pristine NiO epilayers turned to an n-type behavior and the electrical conductivity was increased by one order of magnitude after laser treatment. Photocatalytic activity of the pristine (p-NiO/c-YSZ/Si) and the laser-annealed (n-NiO/p-NiO/c-YSZ/Si) heterostructures were assessed by measuring the decomposition rate of 4-chlorophenol under UV light. The enhanced photocatalytic efficiency was attributed to the suppressed charge carrier recombination in the NiO based p-n junctions and higher electrical conductivity.

Interfacial Modeling and Photochemical Properties of Rutile TiO2/Sapphire Epitaxial Heterostructures: *Mohammad Reza Bayati*[1]; Roya Molaei[1]; Roger Narayan[1]; Jay Narayan[1]; [1]North Carolina State University

TiO2 epitaxial thin films were integrated with on c-sapphire, m-sapphire, and r-sapphire substrates. Using XRD (?/2? and f scans) technique, the epitaxial alignment at the film/substrate interfaces was established as [001](100)rutile||[10-10](0001)c-sapphire, [010](001)rutile||[0001](10-10)m-sapphire, and [010](101)rutile||[2-1-10](01-12)r-sapphire. Based on our STEM results, it was found that the rutile film initially grows pseudomorphically on sapphire as Ti2O3 and, after a few monolayers, it grows tetragonally on the Ti2O3/sapphire platform. Formation of the Ti2O3 transition layer was attributed to the symmetry and chemistry mismatch between tetragonal structure of

TiO2 and hexagonal structure of alumina. In addition, the decomposition rate of 4-chlorophenol by the rutile/sapphire heterostructures under ultraviolet illumination was measured. The relative photocatalytic activity of different faces of rutile TiO2 was shown to be in the following sequence: (001) > (101) > (100). The difference in the photochemical characteristics was attributed to the atomic arrangement on different crystallographic surface planes.

Inverse Spin Hall Effect Studies on ZnO Thin Films: *Megan Prestgard*[1]; Gene Siegel[1]; Shiang Teng[1]; Ashutosh Tiwari[1]; [1]University of Utah
In this talk we will present our work on the inverse spin Hall Effect (ISHE) in ZnO thin films. ISHE refers to the generation of an electric voltage from a spin-current. Although it is a well-studied effect, ISHE has never been investigated in ZnO. For testing ISHE in ZnO films, we designed a novel test structure consisting of a ZnO thin film channel deposited over sapphire substrate, an intermediate MgO tunnel barrier, and a top NiFe layer. The MgO tunnel barrier allows a spin-current to be injected from the NiFe to the ZnO as confirmed by Hanle measurements. A keithley nanovoltmeter was used to measure voltage in ZnO in a direction perpendicular to both the injected spin-current and the spin-direction of the injected carriers. Measurement of this voltage sheds light on the extent of ISHE and stands to establish the potential of ZnO in a wide array of spintronics applications.

Microstructure and 9MeV Au+ Irradiation Effects of 9Cr-ODS(Oxide Dispersion Strengthened) Steel: *Chenyang Lu*[1]; Lumin Wang[1]; Zheng Lu[2]; [1]University of Michigan; [2]Northeastern University
A kind of 9Cr-ODS(oxide dispersion strengthened) steel was produced by mechanical alloying and spark plasma sintering(SPS) at Northeastern University in China. The nominal composition of the steel is Fe-9Cr-1.5W-0.4Mn-0.1Ta-0.2V-0.3Ti-0.3Y2O3 (wt.%). Au+ ion irradiation was carried out using the 9MeV Tandem accelerator at University of Tennessee. The samples were irradiated at 673K to an ion fluence of 7×1016 ion/cm2. The predicted irradiation depth and displacement damage were calculated by the SRIM08 code. Focused ion beam (FIB) lift-out method was adopted for the preparation of cross-section TEM specimen by using a FEI Helios Nanolab Dualbeam. STEM analysis was conducted using a 200kV JEOL 2100F spherical aberration (Cs)-corrected Analytical Electron Microscope, including high angle annual dark field(HAADF) and bright field-STEM imaging techniques. Atom probe tomography (APT) was used to characterize the nano precipitates in the steel.

Observation of the Spin Seebeck Effect in $La_{1-x}Sr_xMnO_3$ (LSMO): *Gene Siegel*[1]; Megan Prestgard[1]; Julia Russ[2]; Ashutosh Tiwari[1]; [1]University of Utah; [2]Ithaca College
LSMO is often used in spintronics research as a spin-injection material. Most commonly, spin-injection is done via spin-polarized electric current passing into a material. In this paper we show the possibility of thermally-induced spin current by means of the spin Seebeck effect (SSE) in LSMO for use in spintronic research and devices. The SSE separates spins in a magnetic material along the direction of a thermal gradient. If a conductor is attached anywhere along the magnet, a pure spin current will flow from the magnet into the metal due to diffusion. This thermally-induced spin current can be detected using the inverse spin Hall effect (ISHE) which generates an electronic current perpendicular to the injected spin current within a strongly spin-orbit coupled material, in this case, platinum. The electronic current is easily measured using traditional electronic measurement tools, and is directly proportional to the amount of spin current that was injected.

Resistance Switching Properties and Mechanism of Switching In Epitaxial Pt/ZnO/TiN Thin Film Heterojunctions Grown on Si(001) Substrate: *Sandhyarani Punugupati*[1]; Jagdish Narayan[1]; Frank Hunte[1]; [1]North Carolina State University
Zinc oxide (ZnO) is a wide band gap semiconductor with applications ranging from opto-electronics, spintronics to memristor based devices. The physical properties of ZnO films are highly sensitive to the growth parameters. We deposited epitaxial ZnO thin films on Si(001) substrate with titanium nitride (TiN) buffer layer using pulsed laser deposition (PLD) technique. To measure the electrical properties, we deposited Pt electrode on ZnO/TiN/Si by PLD using metal shadow mask technique. XRD 2? and f scans indicated that all the films are epitaxial in nature with fixed out of plane orientations. HRTEM images indicated that there was no reaction between various layers. We observed room temperature bi-polar resistance switching in our heterojunctions. These shown reproducible switching up to 24 cycles. We will investigate and present the mechanism of switching in the heterojunctions by imaging them using HRTEM and measuring the junction resistance as a function of temperature.

Structural, Optical and Transport Properties of Room Temperature Deposited Al and Ga Doped ZnO Films: *Namik Temizer*[1]; Sudhakar Nori[1]; Jagdish Narayan[1]; [1]North Carolina State University

Here, we present interesting structural, optical, transport and magnetic properties of Al and Ga doped ZnO films deposited on sapphire and glass substrates at room temperature. The important feature of the current investigation is to obtain films grown at relatively low temperatures that are both conducting and exhibit high transparency (>80%). Low temperature processing is essential (i) to grow films with less strain due to minimized thermal misfit and (ii) for some flexible polymer-based substrates that are heat intolerant. We have found that the microstructure varies from amorphous to nano-crystalline in the above films. The films deposited at higher partial pressure of oxygen show semiconducting behavior, whereas the films grown at lower ambient oxygen partial pressures ($>1x10^{-3}$ Torr) show metal-like behavior with a resistivity minimum. The formation of oxygen vacancy-Zinc interstitial defect complex (V_O-I_{Zn}) could be responsible for the enhancements in n-type conductivity, optical transparency and room temperature ferromagnetism.

Thin Film Epitaxy and Stress Relaxation Mechanism in Rutile/Sapphire Heterostructures: *Mohammad Reza Bayati*[1]; Roya Molaei[1]; Roger Narayan[1]; Jay Narayan[1]; [1]North Carolina State University

We grew TiO2 epitaxial thin films on Al2O3(0001), Al2O3(10-10), and Al2O3(01-12) substrates and studied structure and properties of the epilayers as a function of the crystallographic characteristics of the substrate. The epitaxial relationship across the film/substrate interfaces was determined to be [001](100)rutile||[10-10](0001)c-sapphire, [010](001)rutile||[0001](10-10)m-sapphire, and [010](101)rutile||[2-1-10](01-12)r-sapphire. Our HRTEM imaging and diffraction studies confirmed the established epitaxial alignments and revealed formation of atomically sharp interfaces. The origin and the relaxation mechanism of stress and strain for each heterostructure were studied in detail. It was revealed that large lattice misfit strains relax easily even if the primary slip system is not active. We also showed that even small misfit strains can relax provided that the primary slip system is active. The origin of the residual strains in the epilayers was found to be primarily due to thermal misfit and defect/impurity strains.

Variable Range Hopping Conduction and Magnetic Properties of Single Crystal Semiconducting and Topological Insulator Sr3SnO: *Yi-Fang Lee*[1]; Jagdish Narayan[1]; Justin Schwartz[1]; [1]North Carolina State University

We report epitaxial growth of topological insulator candidate Sr3SnO (SSO) integrated with Si (001) using cubic yttria-stabilized zirconia (c-YSZ) as buffer. X-ray f-scans demonstrated the heteroepitaxial relationship as (001)[100]SSO¦(001)[100]c-YSZ¦(001)[100]Si which was further confirmed by electron diffraction patterns. The electrical resistivities have been measured over a wide range of temperature (5-285K), suggesting semiconductor behavior. The charge transport mechanism was well described by the Variable-Range-Hopping (VRH) law. In particular, two distinct temperature behaviors of resistivity, i.e., the Mott VRH hopping law ln? ? (1/T) 1/4 and the ES VRH hopping law ln? ? (1/T) 1/2 are observed sequentially in appropriate temperature ranges. The hopping conduction parameters such as the characteristic temperature (T0), hopping distance (R), hopping energy (E) and density of states at Fermi level (N(EF) have been calculated. We found room temperature ferromagnetism (RTFM) in SSO, which possess a high saturated magnetization, and a finite non-zero coercivity persisting up to RT.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Nanoceramics I--Nanostructured Ceramics-oxides and Thin Film Interfaces
Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Tuesday 8:30 AM
February 18, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Justin Schwartz, North Carolina State University; Haiyan Wang, Texas A&M University

---

8:30 AM Invited

Resistive Switching Characteristics of Mixed Oxides: *Ram Katiyar*[1]; Rajesh Katiyar[1]; Shojan Pavunny[1]; Geetika Khurana[1]; Pankaj Misra[1]; [1]University of Puerto Rico

We have studied resistive switching phenomenon in mixed oxides, namely ternary oxides LaGdO3 and LaLuO3, multi-ferroic BiFeO3 and Graphene Oxide thin films. Except for the last one, we observed unipolar resistive switching with well defined switching voltages with initial forming process. Forming free bipolar switching was observed in case of Graphene Oxide. The switching mechanism in unipolar cases was found to follow formation of metallic filaments through the agglomeration of oxygen vacancies and metal atoms in films and their subsequent rupture on application of suitable bias voltages. While in case of Graphene Oxide it is believed to be due to the movement of oxygen ions from the bottom ITO electrode into the film and vice versa. The ratio of high and low resistance states was found to be much higher in case of unipolar switching compared to the case of bipolar switching. Details of these results will be presented.

8:50 AM Invited

Growth of Multiferroic Thin-film Heterostructures: *John Prater*[1]; Srinivasa Rao[2]; Sudhakar Nori[2]; Jagdish Narayan[2]; [1]U.S. Army Research Office; [2]North Carolina State University

Different approaches to strain engineering will be discussed in the context of the epitaxial growth of multiferroic thin-film heterostructures. The challenge is especially great for the case of growing these systems epitaxially on Si (100) substrates where large lattice-constant and thermal-expansion mismatches can lead to large residual strains. We report on the heteroepitaxial growth by pulsed laser deposition of various combinations of the multiferroic BiFeO3, and ferromagnetic La0.7Sr0.3MnO3 and Ni82Fe18 (permalloy, Py) thin films, which have been integrated on Si (100) substrates using epitaxial buffer layers of SrTiO3 and MgO/TiN. Approaches to controlling the strains arising from lattice mismatch, thermal mismatch and defect generation will be discussed. Structural and magnetic properties of these layered heterostructures will be presented.

9:10 AM Invited

Oxides for Spintronics: *Ashutosh Tiwari*[1]; [1]University of Utah

Spintronics represents a new paradigm of electronics that utilizes both the electron's charge as well as its spin. It has the potential to facilitate a new generation of logic and photonic devices having high-speed, large memory and ultra-low power consumption. The critical step in the functioning of a spintronic device is the injection and detection of spin-polarized carriers at the ferromagnet-semiconductor interface. Despite considerable efforts, efficient injection of spins into nonmagnetic semiconductors continues to be a major hurdle in this field. All the possible routs of injecting spin in semiconductors rely on oxides. In this talk, I will present some of our very exciting research going on in this field in my group at the University of Utah. Particular focus will be on the injection of spin-polarized carriers in semiconductors using electrical and thermal routes. Acknowledgements:Financial support from NSF through CEMRI Grant#1121252 and CAREER Grant#0746486 is thankfully acknowledged.

9:30 AM Invited

Oxide Based Thin Films, Properties and the Role of Defect Mediation: *Sudhakar Nori*[1]; Jagdish Narayan[1]; [1]North Carolina State University

Although oxides and oxide based thin film systems are widely studied topics in general, yet they continue to surprise periodically by exhibiting interesting physical properties requiring newer insights in order to understand these properties in detail. This talk focuses on the interesting physical properties exhibited by oxide based thin film systems, namely, zinc oxide, vanadium oxide and other rare-earth based manganite heterostructures and the source of origin to some of these striking features such as room temperature ferromagnetism. Point defects like oxygen and zinc vacancies and interstitials are created during the non-equilibrium growth process of the ZnO films. Defect mediation occurs via the formation of oxygen vacancy-zinc interstitial defect complex (V_O-I_{Zn}) that acts as a source of n-type conductivity while the oxygen and zinc vacancies result in the observed ferromagnetism by forming bound magnetic polarons.

9:50 AM

Tunable Magnetotransport and Device Application through Controlling Structural Boundaries in Self-assembled Vertically Aligned Nanocomposite Thin Films: Wenrui Zhang[1]; Aiping Chen[1]; Quanxi Jia[2]; Judith MacManus-Driscoll[3]; *Haiyan Wang*[1]; [1]Texas A&M University; [2]Los Alamos National Lab; [3]University of Cambridge

Vertically aligned nanocomposite (VAN) thin films have recently served as an intriguing platform for obtaining significant understanding of the fundamental physics and exploring novel functionalities for potential technological applications. In this work, the magnetotransport properties of (La0.7Sr0.3MnO3)1-x:(ZnO)x (LSMO:ZnO) VAN films have been systematically investigated through varying underlying substrates and film compositions. The tunability and enhancement of their low-field magnetoresistance (LFMR) have been attributed to controllable grain and phase boundaries, which would greatly affect the formation of electron transport channels. Moreover, the heteroepitaxial LSMO:ZnO VAN films with comparable LFMR properties have been successfully integrated on silicon substrates, which is a critical step enabling the application of VAN films in future spintronic devices. The above results demonstrate that VAN architectures with unique microstructure and interfacial couplings could provide powerful ways for manipulating functionalities in oxide thin films.

10:10 AM Break

10:30 AM Invited

Misfit Accommodation in Oxide Heterostructures: *Matthew Chisholm*[1]; Honghui Zhou[2]; Stephen Pennycook[1]; Jagdish Narayan[3]; [1]Oak Ridge National Laboratory; [2]University of Illinois at Urbana-Champaign; [3]North Carolina State University

We have conducted a detailed structural and spectroscopic study of VO2/NiO/Al2O3 heterostructures using aberration-corrected scanning transmission electron microscopy. Domain matching epitaxy appears to explain the NiO/Al2O3 interface, where we found 12 planes of NiO matching with 13 planes of Al2O3. The VO2/NiO interface is seen to be more complicated with transition region that is structurally and electronically distinct from both the NiO and VO2 films. In this transition region, the crystal structure of the growing vanadium oxide film adopts that of the underlying NiO layer. We find the oxidation state of vanadium increases from ~ 3+ to ~ 4+ with thickness, accompanied by increasing lattice disorder. Reasons for the two different interface reactions will be discussed. This study reveals an important aspect of vanadium oxide growth, i.e., the adaptive growth of an interface mediated phase that assists the structure transition at the VO2/NiO interface.

10:50 AM Invited

Synchrotron Scattering Studies of the Metal-insulator Phase Transition and Local Domain Formation in VO_2: *John Budai*[1]; Jonathan Tischler[2]; Alexander Tselev[1]; Andrei Kolmakov[3]; Olivier Delaire[1]; Michael Manley[1]; Eliot Specht[1]; Ayman Said[2]; Lynn Boatner[1]; Jagdish Narayan[4]; [1]Oak Ridge National Laboratory; [2]Argonne National Lab; [3]Southern Illinois Univ.; [4]North Carolina State Univ.

Synchrotron x-ray facilities now provide a powerful suite of high-resolution tools for investigating local lattice structure and dynamics in nanostructured materials. We have combined several scattering techniques, including scanning microdiffraction, inelastic, and diffuse scattering to study phase evolution and domain formation inside VO_2 microcrystals and epitaxial films. Vanadium dioxide has attracted considerable interest both for device applications and as an important model system for understanding coupled structural and electronic metal-insulator transitions. At ~67°C, the VO_2 resistivity changes by ~4 orders of magnitude and the lattice changes from tetragonal to monoclinic (M1). In addition, applied strains are known to significantly impact the lattice structure, and monoclinic (M2) or triclinic VO_2 phases can also be stabilized. Our scattering studies reveal how domain formation, interface orientations, strain distributions and lattice vibrations near the phase transition depend critically on external and internal stresses. Research supported by Materials Sciences and Engineering Division, U.S. DOE-BES.

11:10 AM Invited

Magnetic Spinel Ferrite Thin Films and Nanostructures: *Arunava Gupta*[1]; [1]University of Alabama

There is considerable interest in spinel ferrite films because of their numerous technological applications in areas such as microwave integrated devices and magnetoelectric coupling heterostructures. The growth and properties of epitaxial spinel ferrite films will be reviewed, including our work on films grown by pulsed laser deposition and chemical vapor deposition techniques. Of particular interest are systematic studies on formation of antiphase boundaries in epitaxial NiFe2O4 films grown on different substrates and the accurate determination of the band gap of this material using optical spectroscopy and first principles calculations. In addition to thin films, spinel ferrite nanostructures are being investigated both because of fundamental scientific interest and technological applications arising from the unique properties in reduced dimension. We have synthesized monodisperse nanocrystals and nanostructures of a number of spinel ferrites using facile solution-based methods and investigated their structural and magnetic properties.

11:30 AM Invited

Routes to Low Defect Interfaces between rocksalt Oxides and Wurtzite Nitrides: Elizabeth Paisley[1]; Benjamin Gaddy[1]; James LeBeau[1]; Christopher Shelton[1]; Ramón Collazo[1]; Zlatko Sitar[1]; *Douglas Irving*[1]; Jon-Paul Maria[1]; [1]North Carolina State University

Low defect heteroepitaxial integration of oxide/nitride polar materials could enable novel functional electronics. In this talk we present results of density functional theory (DFT) integrated with experiment and characterization to investigate mechanisms important to the deposition of low defect (111) oriented rocksalt MgO, CaO, and $Mg_xCa_{1-x}O$ (MCO) onto (0001) oriented wurtzite GaN. Typically, high surface energy of the (111) polar orientation leads to faceting of the oxide and a highly defective thin film. This is overcome by use of a novel molecular beam epitaxy synthesis method that uses H2O as the source of oxygen. Structural characterization by STEM indicates that a finite number of defects persist. DFT results determine the growth window to enable low defect integration, rotational preferences of the MCO on GaN, atomistic mechanisms for persistence of defects in lattice matched MCO films, and electronic properties of the MCO/GaN interface. This work is supported through NSF grant DMR-1151568.

11:50 AM

Simplex Network Modeling for Press-molded Ceramic Bodies Incorporated with Granite Waste: *Leonardo Pedroti*[1]; [1]UENF

Brazil is one of the largest producers and exporters of ornamental rocks in the world. Among them, stands the marble, granite itself, diorite, and gneiss, commercially known as granite and marble. The state of Espirito Santo is the main hub of the country stone installed in the region of Cachoeiro. Formed by a very fine powder, the waste generated by processing, is a major environmental problem. In this work were added different proportions of the sticky residue granite, comprising diamond wire on concrete for evaluation of mechanical properties, chemical and environmental assessed by the determination method simplex from a stroke cement using standard CP-V, the results demonstrate that the residues added to enhance some ratios the characteristics of the mixture, which help to reduce the environmental impact.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Nanometals I-Twinning and Interfacial Effects for Application

Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Tuesday 2:00 PM
February 18, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Xiaozhou Liao, University of Sydney; G. Sundararajan, ARCI

2:00 PM Invited

Radiation Damage Tolerant Nanomaterials: *Amit Misra*[1]; [1]Los Alamos National Laboratory

An overview of the role of the structure and chemistry of interfaces in controlling the radiation damage tolerance of nanomaterials will be presented. A variety of interfaces in model systems were investigated via ion irradiation: grain boundaries in pure metals, and interphase boundaries in fcc-bcc metallic composites and metal-oxides and oxide-oxide composites.Helium ion implantation experiments were used to investigate the storage of stable nano-clusters of helium at interfaces, whereas helium as well as heavy ion irradiation experiments were used to study the evolution of radiation-induced-defect clusters in the vicinity of interfaces. The structural parameters of the interfaces are quantitatively correlated with the accumulation or removal of defects at interfaces. This research is funded by US DOE, Office of Basic Energy Sciences, Energy Frontier Research Center.

2:20 PM Invited

Consequences of Neutron Irradiation on ECAP Steel: *Ahmad Alsabbagh*[1]; Ruslan Valiev[2]; K.L Murty[1]; [1]North Carolina State University; [2]Ufa State Aviation Technical University

Effects of neutron radiation exposure on microstructure and mechanical properties are examined on ultra-fine grained (UFG) carbon steel following equal channel angular processing. Corresponding studies are made on conventional grain (CG) sized material. Radiation hardening and embrittlement were noted in the conventional grain sized steel while relatively small changes were noted in UFG steel. In addition, grain size was noted to increase in the conventional grain sized steel in contrast to no significant effect in the UFG material. Work is in progress to investigate the radiation tolerance of UFG steel at higher fluences.Research is supported by ATR NSUF.

2:40 PM Invited

Laser-accelerated thin foil impact experiments for studies of intermetallic reactions in Nanolayered Ni+Al foils: Sean Kelly[1]; *Naresh Thadhani*[1]; [1]Georgia Institute of Technology

Shock-compression of fully-dense nano-Ni+Al multi-layered foils is investigated to probe the occurrence of shock-induced intermetallic-forming reactions. A laser-accelerated thin flyer impact system was utilized to determine the shock equation-of-state of the nano-layered Ni+Al foils. Measurements performed using time-resolved VISAR and PDV interferometry, showed evidence of shock-induced reaction based on change in the slope of the shock versus particle velocity response at pressures > 5 GPa, with recovered samples also clearly exhibiting a self-sustained reaction. Post-mortem high-resolution transmission electron microscopy (HRTEM) confirmed the formation of B2-NiAl in the reacted samples, and samples impacted at shock pressures below the reaction threshold revealed evidence of reactant mixing in regions close to heterogeneities associated with the wavy nature of the nano-layers. In this presentation, the mechanics of nano-layer deformation and strain localization at heterogeneities, leading to reaction initiation will be described.

3:00 PM

The Surface Energy of the Al-Cu-Fe Quasicrystal: *Jean-Marie Dubois* ; Institut Jean Lamour

Application niches for quasicrystalline thin films or coatings were pointed out in the areas of thermal insulation, infrared absorption, and reduced friction and adhesion, which led the author to be honored by the 2007 Mehl Award. Hence, attempts were made to estimate the surface energy (?S) of the stable i-Al62Cu25Fe13 (at.%) quasicrystal. Pin-on-disk experiments, after appropriate calibration, lead to reliable data in the range 0.5<?S<0.8Jm-2. Confirmation that ?S lies in this range is provided by indirect measurements, based on the formation of composites made of blends of i-AlCuFe with immiscible metals like Sn and Bi. The average value of ?S is about one half of that of pure aluminum (?S=1.15-1.2Jm-2), and less than a quarter of that of iron (?S=2.2-2.4Jm-2, consistently with the low wetting behavior and reduced friction coefficient observed for this quasicrystal. Correlation to specific features of the DOS will be emphasized.

3:20 PM Break

3:40 PM Invited

Atomic-scale Understanding of Deformation Twins in Hexagonal-close-packed Metals: *Jian Wang*[1]; Carlos Tome[1]; Irene Beyerlein[1]; John Hirth[1]; [1]Los Alamos National Laboratory

Deformation twinning/de-twinning, which are the dominant deformation mechanisms in hexagonal-close-packed (HCP) metals, exhibit more complex nucleation and propagation mechanisms than those associated with dislocation slip and those in cubic structures (FCC and BCC). Specifically, twinning and de-twinning are directional, involve atomistic shuffling, and they induce a strong crystallographic reorientation. Twin nucleation, a necessary first stage of twinning, seems to invariably take place at grain boundaries in hcp materials, and to involve complex dislocation reactions. After twin nucleates, propagation, growth, and interactions of twins seem more complicated than that in cubic crystals. In this talk, I will focus on the fundamental understanding of the aforementioned processes based on HRTEM observations and atomistic simulations. The fundamental mechanisms, including pure-shuffle, glide (shear)-shuffle and climb-shuffle, will be discussed in association with twinning and de-twinning.

4:00 PM Invited

Deformation Twinning and De-twinning in Nanostructured Materials: *Xiaozhou Liao*[1]; [1]The University of Sydney

Recent investigations indicated that increasing the density of twin boundaries can effectively strengthen materials and at the same time retain or improve their ductility because twin boundaries impede dislocation slip and also increase the dislocation storage capability in materials. Plastic deformation is a rapid and efficient way to produce a very high density of twins with twin boundary spacings in the nanometre regime in materials. In many situations, deformation can also lead to de-twinning. In this presentation, I will discuss our experimental observations of (1) the mechanisms of deformation twinning and de-twinning and (2) the effects of stacking fault energy, grain size and applied pressure on the twinning and de-twinning behavior in nanostructured materials.

4:20 PM Invited

Switchable Deformation Mechanism in Columnar-grained Nanotwinned Metals: Zesheng You[1]; Xiaoyan Li[2]; Ting Zhu[3]; Huajian Gao[2]; *Lei Lu*[1]; [1]Institute of Metal Research, CAS; [2]School of Engineering, Brown University; [3]Woodruff School of Mechanical Engineering, Georgia Institute and Technology

Nano-scale twin strengthening represents a powerful strategy of achieving unprecedented mechanical properties (e.g., ultrahigh strength, high ductility, facile damage and flaw tolerance) in engineering metals and alloys. However, it has not been possible to tailor-design the nanostructures and associated properties in nano-twinned materials for obtaining targeted properties in a controlled manner. In this work, by integrating the nanostructure processing and characterization, we show that the strength and strain hardening properties can be tailored to vary over a large range in a columnar-grained nano-twinned copper simply by changing the loading orientations. We find such versatile performance can be achieved in a single nanostructured system owing to the switchable deformation mechanisms among different hard and soft modes of dislocation-mediated plasticity. Such switchable mechanisms are attributed to the unique layered organization of nanoscale twin lamellas in the columnar grains as well as the facile plastic shear mechanisms mediated by the coherent twin interfaces.

4:40 PM Invited

Deformation Twinning in Nano-scale Cu Layers: Rodney McCabe[1]; *Irene Beyerlein*[1]; John Carpenter[1]; Shijian Zheng[1]; Nathan Mara[1]; [1]Los Alamos National Laboratory

We examine twinning statistics in nano-layered Cu/Nb composites produced by accumulative roll bonding (ARB) using a novel, high spatial resolution electron backscatter (EBSD) technique. Below average layer thicknesses of 100 nm, twinning becomes an important deformation mode in the Cu layers. We reveal a significant orientation dependence, in which twinning is prevalent in Cu grains with certain orientations and rare for others despite similar strain histories and grain sizes. We develop a theoretical model that captures the favorability of twinning versus slip with crystal orientation. Interestingly, our results indicate that the size effects observed in nano-scale fcc metals are as much a consequence of crystal orientation and the large stresses as they are an inherent result of crystal size. We also quantify the effects of twinning on the evolving Cu texture and related interface characters present in the composites.

5:00 PM

Basic Criteria for Formation of Growth Twins in High Stacking Fault Energy Metals: *Xinghang Zhang*[1]; Kaiyuan Yu; Daniel Bufford; Yue Liu; Youxing Chen; Haiyan Wang; [1]Texas A&M University

Nanotwinned metals received significant interest lately as twin boundaries may enable simultaneous enhancement of strength, ductility, thermal stability and radiation tolerance. However nanotwins have been the privilege of metals with low-to-intermediate stacking fault energy (SFE). Recent scattered studies show that nanotwins could be introduced into high stacking fault energy (SFE) metals, such as Al. In this talk we review several sputter-deposited (111) textured Ag/Al, Cu/Ni and Cu/Fe multilayers, wherein growth twins were observed in Ni, Al and face-centered cubic (fcc) Fe. The comparisons lead to important design criteria that dictate the introduction of growth twins in high SFE metals. The validity of these criteria was then examined in Ag/Ni multilayers.

5:20 PM

The Influence of Stacking Fault Energy on the Formation of Highly Nanotwinned Cu-Al Alloys: *Leonardo Velasco*[1]; Mikhail Polyakov[1]; Andrea Hodge[1]; [1]University of Southern California

Thin films of pure Cu (99.999%) and Cu-Al alloys (Cu- 6 wt.% Al and Cu- 4 wt.% Al) were sputtered under identical conditions, in order to compare nanotwinned microstructures. Due to the wide range of stacking fault energies (SFE) in these materials (6-78 mJ/m2), the microstructure features were expected to change substantially. The temperature during processing was measured in order to explore and understand the different sputtering behavior for Cu and Cu-Al alloys and its influence on generating a nanotwinned structure. The samples produced were characterized by TEM and FIB. The Cu-Al samples showed highly columnar and nanotwinned structures, while the Cu samples presented few columnar grains, limited number of nanotwinned grains, and fine grain size. The reduced SFE of the Cu-Al alloys promoted a highly aligned nanotwinned columnar grain structure.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Nanometals II-Processing and Strengthening Mechanisms
Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Wednesday 8:30 AM
February 19, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Evan Ma, Johns Hopkins University; Suveen Mathahaudhu, US Army Research Office

---

8:30 AM Invited
Superior Strength in Bulk Nanostructured Metallic Materials Produced by SPD Processing: *Ruslan Valiev*[1]; Nariman Enikeev[1]; Sergei Firstov[2]; [1]Ufa State Aviation Technical University; [2]Frantsevich Institute for Problems of Materials Science
Recent studies demonstrated that the processing of metallic alloys by severe plastic deformation (SPD) can result in not only strong grain refinement but also different phase transformations dealing with second phase dissolution, formation of grain boundary segregations and precipitations. These nanostructural features of SPD-processed alloys produce considerable influence on their mechanical properties. The report presents experimental data and modeling results demonstrating “positive” slope of the Hall-Petch relation when passing from micro- to nanostructured state in a number of metallic materials subjected to SPD. The observed extra-strength is related to the changes in strengthening mechanisms of ultrafine-grained materials as a result of changes in grain boundaries structure. The nature of superior strength is associated with the difficulty of generation of dislocations from grain boundaries with segregations. This new approach is used for achieving the enhanced strength in several commercial Al and Ti alloys as well as steels subjected to SPD processing.

8:50 AM
Dynamic Strain Aging in Ultrafine Grained Titanium: *Felipe Lopes*[1]; Sergio Monteiro[1]; Daniel Fernandes[1]; Carlos Elias[1]; Chia-Hui Lu[2]; Ruslan Valiev[3]; Marc Meyers[2]; [1]IME; [2]UC San Diego; [3]Ufa State Aviation Technical University
Titanium and its alloys are very important for the industries and medicine, because of the properties, mainly corrosion resistance, lightweight, strength and biocompatibility. This new titanium was processed by ECAP-Conform, with this new structure the strength was improved and some authors say that UFG Ti is stronger than its alloys commonly used, for example: Ti-6Al-4V, but it’s not true at all. UFG Ti is stronger in comparison with this alloy, just in some range of strain rate, exactly, when happens the dynamic strain aging (DSA), it's necessary to understand better the phenomenon. The objective of this paper was investigate into which range of strain rate and temperature this phenomenon happens by compression tests and indentify the deformation mechanism by TEM. The results show that happens in UFG Ti at $10^{-2.5}$ to $10^{-3.5}$ s^{-1} for room temperature and the deformation mechanism observed by TEM were grain-boundary rotation and perhaps twin bands.

9:10 AM Invited
Generation of Bulk Nanocomposites and Supersaturated Solid Solutions by Severe Plastic Deformation: *Andrea Bachmaier*[1]; Anton Hohenwarter[2]; Reinhard Pippan[3]; [1]Saarland University; [2]University of Leoben; [3]Austrian Academy of Sciences
Severe plastic deformation (SPD) can be used to produce ultrafine grained materials from nearly all kind of bulk coarse grained metal materials. This work is devoted to the generation of nanocomposites and stable nanocrystallites by SPD. A High-Pressure Torsion (HPT) powder compaction technique permits the generation of nanocrystalline

composite materials with enhanced thermal stability. During HPT of composites or powder mixtures, the formation of supersaturated solid solutions or even amorphization reactions can occur in alloys with a positive heat of mixing ?H due to a kind of “mechanically alloying in bulk form”. Nanometer sized grains are reported to be a basic requirement to obtain supersaturated solid solutions. Hence, a novel two-step HPT powder consolidation and deformation process was developed, which has an increased effectiveness compared to conventional ones. During annealing, the supersaturated solid solutions decompose and form two-phase nanostructured composites with an enhanced hardness and an improved thermal stability.

9:30 AM Invited

Crystallization of Metallic Glasses to Produce Nanostructured Materials: *Ken Kelton*[1]; [1]Washington University

Metallic glasses are increasingly finding new applications due to their good corrosion resistance, high yield strength, and other desirable physical properties. In some cases, the properties are further improved by partially crystallizing the glass to form a nanocrystal/amorphous composite. Nucleation and growth during crystallization are often complex, sometimes coupling to structural and chemical ordering in the amorphous phase and to other phase transitions. Knowledge of these processes is necessary if a tailored nanostructure is to be achieved. It is also essential to ensure the stability of the glass or nanocrystal/amorphous composite in the environment of the desired application. A few selected examples of glass and liquid crystallization will be presented to illustrate these points. Partially supported by the NSF (DMR-12-06707)

9:50 AM Break

10:10 AM Invited

A Review of Strengthening Mechanisms in Nanomaterials: *Chandra Pande*[1]; [1]Naval Research Laboratory

Masumura, Hazzledine and Pande (Acta Mater. 46 (1998) 4527) were the first to show that Hall-Petch plot for a wide range of materials and mean grain sizes could be divided into three distinct regimes and also first provided a detailed mathematical model of Hall-Petch relation of plastic deformation processes for any material including fine-grained nanocrystalline materials. In this paper this model is developed further to include nanocomposites and nanomaterials with bimodal grain size distributions. Special attention is paid to the abnormal Hall-Petch relationship, which manifests itself as the softening of nanocrystalline materials for very small (less than 12 nm) mean grain sizes. It is shown that the modeling the strength of nanocrystalline materials needs consideration of both dislocation interactions and sliding. Such a model appears to be most successful in explaining experimental results in a variety of nanomaterials.

10:30 AM Invited

Industrially Useful Nanostructured Molybdenum Alloys with Unprecedented Tensile Ductility: *Evan Ma*[1]; [1]Johns Hopkins University

The high-temperature stability, creep resistance, thermal conductivity of refractory molybdenum alloys are highly desirable for a wide range of applications. But molybdenum alloys are also a well-known example of body-centered-cubic materials that suffer from low ductility and limited formability. In collaboration with J. Sun (XJTU) we solve this long-standing problem via a new nanostructuring route that optimizes the distribution of the grains, strengthening dispersions and solutes (G. Liu et al., Nature Materials, 2013). A simple and cost-effective molecular-level liquid-liquid mixing/doping technique is developed to achieve ultrafine submicron-sized grains with nanosized oxide particles uniformly distributed in the grain interior. The resulting hybrid Mo alloys boast an extraordinary tensile elongation as large as ~40% at room temperature. The new processing route is used for large-scale industrial productions of ductile Mo alloys that can be extensively shaped. Our findings can be used for engineering dispersion-strengthened architectured materials with simultaneously high strength and ductility.

10:50 AM Invited

High-strength Low-alloyed Zinc Processed by High-pressure Torsion: *Javier Gil Sevillano*[1]; Tobias Zühlke[1]; Jon Iglesias Erausquin[1]; Jon Alkorta[1]; Heinz Werner Höppel[2]; Mathias Göken[2]; [1]CEIT and TECNUN, University of Navarra; [2]University of Erlangen-Nuremberg

Coarse grain pure zinc and a low-alloyed zinc EN988 (0.16 % Cu, 0.08% Ti, in mass percent) have been processed by high-pressure torsion (HPT) up to very high plastic deformation (equivalent true strain: 400) at room temperature. Pure zinc undergoes a discontinuous dynamic recrystallization and reaches early a steady state of relatively coarse heterogeneous structure (˜15 µm) and low strength (130 MPa). By contrast, the zinc alloy undergoes a process of dynamic continuous recrystallization that induces a homogeneous sub-micron grain structure (˜150 nm) and a persistent strengthening up to a true equivalent strain of 300, reaching a maximum strength of about 700 MPa. The origin of such unusual strengthening is discussed on account of both the evolution of the crystallographic texture and grain size, and the influence of the small volume fraction of TiZn16 second phase present in the alloy during the HPT process.

11:10 AM Invited

Finding Strength in Our Faults: Extreme Strengthening of Mg-alloys via Nano-spaced Stacking Faults: Weiwei Jian[1]; Weizhong Xu[1]; Hao Yuan[1]; Ming-Hung Tsai[1]; Carl Koch[1]; Yuntian Zhu[1]; *Suveen Mathaudhu*[2]; [1]North Carolina State University; [2]U.S. Army Research Office

Mg alloys are among the lightest alloys but their strengths are usually low. Here we report a new mechanism to make them ultrastrong and moderately ductile. Stacking faults with nanoscale spacing were introduced into a Mg-8.5Gd-2.3Y-1.8Ag-0.4Zr (wt. pct.) alloy by conventional hot rolling, which produced a yield strength of ~575 MPa, an ultimate strength of ~600 MPa, and a uniform elongation of ~ 5.2%. Low stacking fault energy played an essential role in producing a high density of stacking faults which impeded dislocation slip and promoted dislocation accumulation. These findings provide guidance for development of Mg alloys with superior mechanical properties.

11:30 AM Invited

Microstructural and Geometrical Size Scale Effects in Shape Memory Alloys: *Raj Vaidyanathan*[1]; [1]UCF

Results from microcompression experiments on single crystal micron-scaled pillars of NiTi of known orientations are extended to understand the effect of microstructural length scales and sample geometry on shape memory behavior. The microcompression experiments are supplemented by in situ neutron diffraction measurements at stress and temperature on bulk samples on engineering diffractometers at Los Alamos National Laboratory and Oak Ridge National Laboratory. The samples investigated include binary NiTi samples under isostress, isothermal and isostrain loading conditions and a ternary NiTiHf alloy with a coherent, nano-sized precipitate phase. Conclusions are drawn on the effect of microstructural length scales and sample geometry on the thermoelastic transformation and more specifically their implications on shape memory properties including: the gradient and the hysteresis during the phase transformation, the recoverable strain associated with the transformation and the evolutionary unrecoverable strain with thermomechanical cycling.

11:50 AM

Grain Size Effect on Deformation Physics of Nanostructured Materials: *Yuntian Zhu*[1]; Guangming Cheng[1]; Xiaozhou Liao[2]; Xiaolei Wu[3]; [1]North Carolina State University; [2]University of Sydney; [3]Chinese Academy of Sciences

Grain size has been found to have a significant effect on the deformation physics of nanomaterials and this consequently affects their mechanical behaviors. In this presentation, I'll first present the grain size effect on the deformations physics of nano fcc, hcp and bcc metals. The extensive studies on deformation physics for the last two decades have been focused primarily on the fcc systems. There are still many issues in the bcc and hcp systems to be addressed by our materials community.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Nanomaterials for Device Applications and Nanometal III-Deformation Mechanisms
Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Wednesday 2:00 PM
February 19, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: R. Katiyar, University of Puerto Rico; Somuri Prasad, Sandia National Lab

---

2:00 PM Invited
Nanoengineered Binary and Ternary Heavy Metal Selenides for MWIR Detectors: *Narsingh Singh*[1]; [1]University of Maryland, Baltimore County
A large number of papers have been published in the past fifteen years on the growth and characterization of nanoparticles/nanowires of variety of materials. In spite of huge investment wide applications in systems applications has not been realized. There is a great potential for nanoparticles, nanodots and nanowires for their applications in electronic and optical devices and sensors since nanoparticles have shown that they can amplify the Raman scattering cross section of the molecules absorbed on them. Lead, mercury and thallium selenides have excellent properties for high operating temperature (HOT) mid infrared wavelength (MWIR) and long infrared wavelength (LWIR) detectors. We have performed experiments on the vapor growth of PbSe and HgSe and have demonstrated parameters for oriented nanocrystals on large substrates. We will describe the dependence of growth conditions on the morphology and relevant properties for novel devices and their progress.

2:20 PM Invited
Electronically-active Silicon Nanophotonic Structures for Nonlinear Optics on a CMOS-compatible Chip: *Shayan Mookherjea*[1]; [1]UC San Diego
Traditionally, nonlinear optics conjures images of large vibration-isolated tables, powerful lasers, and painful alignment of optical components with many dozens of degrees of freedom. In contrast, chip-scale nonlinear optics, especially fabricated using CMOS tools in silicon, is stable, energy efficient, scalable and much more compact. This technology can enable practical applications of wavelength conversion, signal processing and quantum science. Here, we will review recent progress made in achieving record performance in classical and quantum optical four-wave mixing using nanostructured silicon photonic chip-scale devices with a few milliwatts of pump power.

2:40 PM Invited
Fabrication, Characterization, and Mechanism of Vertically Aligned Titanium Nitride Nanowires: Seyram Gbordzoe[1]; Mainul Faruque[1]; Kwadwo M-Darkwa[1]; Zhigang Xu; *Dhananjay Kumar*[2]; [1]North Carolina Agricultural and Technical State University; [2]North Carolina A & T State Univ
Titanium nitride (TiN) nanowires have been grown on single crystal magnesium oxide (MgO) substrates using a bottom-up pulsed laser deposition method where Ti-N based gaseous reactants in the laser plume supersaturate the catalytic gold (Au) liquid located on the substrate surfaces. Growth of TiN continues as long as the dissolution rate of material into the catalyst matches the extrusion of solid material at the liquid/solid interface. This bottom-up approach gives rise to a one-dimensional TiN nanowire structure (length: 200-300 nm and diameter: 20-30 nm) capped with a catalytic Au seed. The ascent of Au nanodots to the top of TiN nanowires can be explained based on breaking of weaker bonds and formation of stronger bonds. From strength point of view, these bonds are listed here in order of decreasing strength as follows: Ti-O (672 KJ/mol) > Ti-N (496 KJ/mol) > Au-N (416 kJ/mol) > Au-O (221 kJ/mol). The TiN nanowires were provided vertical alignment by selecting a plane of the substrate that provides the least lattice mismatching to the (111) plane of TiN which has lower surface energy than its other planes: (100) or (110).

3:00 PM Invited

Novel Bimetallic Plasmonic Nanomaterials: *Ritesh Sachan*[1]; R. Kalyanaraman[2]; G. Duscher[2]; [1]Oak Ridge National Laboratory; [2]University of Tennessee

We study Ag-Co bimetallic nanoparticles (NPs) due to its unique plasmonic characteristics. A self-organization route based on pulsed laser induced dewetting of bilayer metallic films is used to synthesize Ag-Co bimetallic plasmonic NPs. The far-field optical results showed that surface plasmon (SP) in Ag-Co NPs can be tuned over a wavelength range one order magnitude greater than that for pure Ag NPs. Ag-Co NPs show a life-time of nearly an order of magnitude higher than pure Ag NPs due to cathodic protection of Ag by galvanic coupling of Ag and Co within the NPs and thus show ultrastable optical properties. With near-field optical analysis by low-loss EELS, first known discovery of strong visible wavelength SP in Co region of bimetallic NPs was made which is unique finding due to well-known highly damped plasmonic nature of pure Co. This discovery is useful for making next generation bio-sensing devices.

3:20 PM

Hollow Fiber Solar Cells: Processing, Morphology, and Property Correlations: Tyler Smith[1]; *Abhinav Malasi*[1]; Hernando Garcia[2]; Gerd Duscher[1]; Ramki Kalyanaraman[1]; [1]University of Tennessee, Knoxville; [2]Southern Illinois University Edwardsville

In the field of photovoltaics, device architecture can play a lead role in increasing the efficiency of solar cells. One promising design is to make inorganic solar cells inside hollow polymer fibers. This geometry allows greater light absorption and increases the ratio of trapping length to recombination length, potentially leading to higher efficiency. This geometry can also result in low cost, lightweight, flexible and efficient solar cells for various applications, including as textiles and large area solar harvesters. In this study, we present results of CdS based Schottky device fabricated using low temperature chemical bath deposition (CBD) technique in planar and hollow fiber configurations. The electrical, optical and I-V characteristics of the Schottky device in correlation to processing and morphology characteristics will be presented. The eventual goal will be to fabricate inorganic heterojunction solar cells inside hollow fibers, enabling a new generation of low cost and high efficiency solar cells.

3:40 PM Break

4:00 PM Invited

The Hall-petch Based Dislocation Mechanics of Nanopolycrystal Plasticity: *Ronald Armstrong*[1]; [1]University of Maryland

The dislocation mechanics aspects of the Hall-Petch based inverse square root of grain size dependence of strength and strain rate sensitivity are described for the range of conventional to nanopolycrystalline metals. Emphasis is placed on connection with the researches of Jay Narayan who has contributed both to the production of nano-materials and to assessment of their properties. Of particular interest here is evaluation of the H-P stress intensity (slope value), k, that is attributed to the requirement of activating secondary prism or pyramidal slip systems in the grain boundary regions of hexagonal close-packed (hcp) metals and of activating cross-slip at the grain boundary regions of face-centered cubic (fcc) metals; thus supplying an explanation of a lowest k value for aluminum at ambient temperature. A lowered value of k for nano-iron and steel materials is attributed to reduction of Cottrell-locking at grain boundary regions and to possible grain boundary disorder.

4:20 PM Invited

Modeling of Grain Boundaries in Nanostructured Alloys: Structure, Stability and Dynamics: Shijing Lu[1]; *Donald Brenner*[1]; [1]North Carolina State University

Addition of solute atoms to nanostructured metals can have a profound influence on stability and mechanical properties. This can result from thermodynamic stabilization from solute segregation, or reduction of grain boundary mobility due to solute drag. We have been using a combination of density functional theory, molecular dynamics simulations and meso-scale defect modeling to better understand how the combined properties of solvent and solute atoms influence grain boundary stability and mobility. Three aspects of this work will be discussed, a perturbation approach that allows rapid calculation of solute substitution energies, simulations of the effect of grain boundary segregate density on grain boundary motion at high driving forces, and simulations combining Monte Carlo and molecular dynamics simulations to model grain boundary mobility at lower driving forces. This work was supported by a grant from the Office of Naval Research.

4:40 PM Invited

The Role of Interfaces on the Deformation Behavior of Nanocrystalline Thin Films and Bulk Materials: *Mathias Göken*[1]; [1]Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Nanocrystalline materials and thin films show a great potential concerning their mechanical properties. Although there mechanical properties have been investigated quite intensively, the role of interfaces on the deformation behavior is still discussed controversially. Investigations of thin Au-films and nanotwinned thin Cu-films with a bulge test inside an atomic force microscope show easy sliding and rotation of columnar grains in the thin films. This interface sliding probably also causes the found extremely low fracture toughness of the thin gold films. These results are in good agreement with nanoindentation experiments on bulk nanocrystalline materials where Focused Ion Beam cross sections clearly reveal sliding of grains out of the free surface. However, underneath the indenter inside the bulk, no direct evidence of interface sliding has been found. Here the constraints imposed from the neighboring grains, limit sliding of interfaces and require dislocation processes to be active during deformation.

5:00 PM Invited

Friction Behavior of Nanocrystalline Metals: The Role of Subsurface Grain Structures: *Somuri Prasad*[1]; Corbett Battaile[1]; Henry Padilla[1]; Brad Boyce[1]; Paul Kotula[1]; [1]Sandia National Laboratories

Tribological behavior nancrystalline alloys (Ni, Ni-Fe, Au) was evaluated under a range of contact stresses and sliding speeds. Friction-induced microstructural changes in the subsurface regions were examined by TEM. At low sliding speeds (or normal forces), the steady-state COF decreased to μ˜0.2 whereas at higher sliding speeds and normal forces, the steady-state COF remained high, μ˜0.8. In cases that exhibited low friction behavior, subsurfaces revealed the presence of ultrafine nanocrystalline zones with 2-10 nm size grains, formed due to friction-induced deformation. We believe that the existence of these ultrafine nanocrystalline layers changed the deformation mechanism from the traditional dislocation mediated one to that predominantly controlled by grain boundaries. The key distinction between the high-friction and low-friction conditions appears to lie in the triggering of a delamination process. Finite element analysis is used to aid in the understanding of how the magnitude and location of stresses drive these two distinct regimes.

5:20 PM Invited

3D TEM Characterization of Nanocrystalline Metal Thin Films: *Xiaoxu Huang*[1]; S. Schmidt[1]; P. Larsen[1]; H. H. Liu[2]; A. Godfrey[3]; Z. Q. Liu[4]; [1]Technical University of Denmark; [2]California Institute of Technology; [3]Tsinghua University; [4]Institute of Metal Research

Characterization of nanocrystalline metal films using transmission electron microscopy (TEM) encounters difficulties to resolve multiple through thickness grains and to provide statistical data of grain orientations and grain boundary characteristics. We have employed a newly developed technique for three-dimensional orientation mapping in the TEM (3D-OMiTEM), which has a spatial resolution of 1 nm, to obtain 3D grain maps of nanocrystalline metal films produced by deposition processes. From the 3D grain maps, structural parameters such as size, shape and crystallographic orientation of individual grains, and normal, curvature and misorientation of grain boundaries in the volume analyzed, can be obtained. In this presentation, examples of 3D grain orientation maps generated from the 3D-OMiTEM are illustrated, showing the importance of using 3D techniques for a precise characterization of structural parameters of nanocrystalline metal films.

2014 TMS RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and Their Applications: Nanomaterials for Energy Applications and Carbon Related Materials
Sponsored by: TMS: Thin Films and Interfaces Committee
Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramki Kalyanaraman, University of Tennessee; Haiyan Wang; Yuntian Zhu, North Carolina State University; Justin Schwartz, North Carolina State University; Amit Goyal, Oak Ridge National Laboratories

Thursday 8:30 AM
February 20, 2014
Room: Ballroom E
Location: San Diego Marriott Marquis & Marina

Session Chair: Nitin Chopra, University of Alabama; Ashutosh Tiwari, University of Utah

---

8:30 AM Invited
Charged Defect-induced Preferential Scattering for Enhanced Thermoelectric Performance in Few-layered n-Bi2Te3: *Apparao Rao*[1]; [1]Clemson University
In the past two decades the development of nano-structuring methods, such as the ball milling-hot pressing, melt spinning-spark plasma sintering, hydrothermal growth-cold pressing, and hot forging processes have improved the figure of merit (ZT) in the state-of-the art bulk thermoelectric (TE) materials. While these methods can enhance the TE performance of p-type Bi2Te3, they proved ineffective for n-type Bi2Te3 due to the inevitable deterioration of its TE properties in the basal plane. Here, we describe a novel chemical-exfoliation spark-plasma-sintering (CE-SPS) nano-structuring process that transforms the microstructure of n-type Bi2Te3 in an exceptional way without compromising its basal plane properties. The CE-SPS processing leads to a significant decrease in the electrical resistivity despite the presence of numerous grain boundaries, mitigates the bipolar effect leading to an upshift of the ZT peak by ~100 K, and stabilizes ZT to a value above 0.8 over a temperature range of ~150 K. The confluence of these highly desirable properties stems from the preferential scattering of electrons at the charged grain boundaries created by the CE-SPS process. In addition, compared to the compatibility factor of the commercial ingot the CE-SPS processed n-type Bi2Te3 exhibits a weak temperature dependence in the range of 300-500 K , thus paving the way for the integration of existing non-traditional TE materials into TE devices.

8:50 AM Invited
Laser Ablation in Liquids: A Unique Route to Fabricate Hollow Micro/Nanoparticles from Bulk Materials: *Douglas Chrisey*[1]; [1]Tulane University
Hollow micro- and nanoparticles are attractive due to the wide range of applications based on their high specific surface area. Laser ablation in liquids has been a subject of intensive research in the past decade, but the particles generated by this method were limited to solid ones. We found that hollow particles could be generated by excimer laser ablation of Al, Cu, Pt, Fe-Ni alloy, TiO2 and Nb2O5 targets in water or aqueous solutions. The hollow particles generally have smooth shells, but may also be aggregated from nano- or even microparticles. Herein we extend the method to other materials and discuss the possibility of laser ablation in liquids as a general approach to fabricate hollow particles directly from bulk materials. The hollow particles are formed on laser-induced bubbles. This mechanism provides the possibility to fabricate hollow particles from other materials and represents a new paradigm for hollow particle fabrication.

9:10 AM Invited
A New Class of Molecularly-tailored Nanomaterials and Interfaces For Energy Conversion and Thermal Management: *Ganpati Ramanath*[1]; [1]Rensselaer Polytechnic Institute
This talk will describe new molecularly-directed synthesis and modification strategies to realize nanomaterials and interfaces for energy and electronics applications. I will first demonstrate a new class of doped-nanothermelectrics obtained by the assembly of surfactant-sculpted nanocrystals of pnictogen chalcogenides and oxides synthesized by a scalable and versatile microwave-solvothermal approach. Sintered nanostructure assemblies exhibit up to 250% higher

figure of merit resulting from nanostructuring-induced ultralow thermal conductivities, and doping-induced enhancements in the power factor through control over charge carrier type, concentration and mobility through alterations in defect chemistry and electronic band structure. Property enhancement mechanisms will be discussed based upon electron microscopy, electron and X-ray absorption spectroscopies and first principles theoretical calculations. I will also demonstrate the ability to tune the interfacial thermal conductance by more than an order of magnitude using a nanomolecular layer that alters the interfacial bond chemistry and the vibrational band structure.

9:30 AM Invited

Atomistic Study of Thermoelectric, Electronic and Optical Properties of Suspended Graphene Nanosheet and Nanoribbons: *Sarang Muley*[1]; Ravindra Nuggehalli[1]; [1]New Jersey Institute of Technology

Non-equilibrium molecular dynamics (NEMD) simulations and Non-Equilibrium Green's Function (NEGF) formalism have been used to investigate and compare the thermoelectric, electronic and optical properties of a series of both suspended pristine as well as p- and n-type doped 1D zigzag and armchair graphene nanoribbons (GNR) with 2D graphene nano-sheets. Thermoelectric and electronic properties are found to exhibit interesting width dependence. Also, these carbon nanostructures could have enhanced thermoelectric figure of merit (ZT) values at appropriate chemically-doped carrier concentration and operating temperature. Significant role of the quasi-1D geometry in determining the thermoelectric properties of the GNR has been observed. Optical absorption coefficient and refractive indices have been found to be independent of chemical doping (upto 12%) and incident wavelength (300-1000 nm) for single and bilayer graphene. Possessing an extraordinary set of properties, these carbon nanostructures can be promising candidates for high performance thermoelectric and opto-electronic devices.

9:50 AM Break

10:10 AM Invited

Does Function Follow Form? The Role and Utility of Geometry in Carbon Nanotubes: *Prabhakar Bandaru*[1]; [1]UC, San Diego

The synthesis of nonlinear morphologies of nanotubes and nanowires, such as branched and coiled forms, has been widely reported and suggests novel applications, e.g., coiled forms for mechanical springs and electrical inductors, and branched structures for interconnect and switching applications, etc. Such nanostructure formation is also scientifically interesting in that nonlinearity abounds in nature, e.g., DNA based structures are often coiled and a connection could be seen to be made at the nanoscale between carbon based inorganic and organic structures. For application, it would be desirable to have control over the nanostructure morphology and geometry-which has not been achieved, due to an incomplete understanding of their growth mechanisms. In this talk, I will briefly review the forms and growth models in vogue, indicating the critical role of the catalyst and growth ambient. I will then discuss experimental results that indicate utility of such morphologies and whether they confer critical advantages.

10:30 AM Invited

Improved Interlaminar/Interfacial Fracture Toughness through Polymer Nano-particle Thin Film/Spray Mediated Composites: *Ranji Vaidyanathan*[1]; Krishna Bastola[1]; [1]Oklahoma State University

Polyhedral Oligomeric Silsesquioxane (POSS), and graphene are classes of nano-sized additives that can potentially compete with techniques to improve the interlaminar/interfacial shear strength of carbon fiber epoxy laminate composites and outperform techniques such as interleaving, stitching, z-pinning, or hybridization with micro or nano-sized particles. The present study was undertaken to explore the possibility of modifying the interlaminar interface of carbon fiber epoxy laminate composites at the nanoscale using POSS or graphene oxide dispersed in a thermoplastic polymer carrier such as polyvinyl pyrrolidone (PVP) or starch and applied in the mid-plane of a composite laminate. Improvement of ~100% in the Mode I fracture toughness (GIc) that was observed makes the technique of using very small amounts of POSS or graphene oxide nano-particles (< 0.5% by weight) to modify interlaminar interface, an innovative means to improve the energy absorption capability and interlaminar shear strength of carbon fiber epoxy laminates.

10:50 AM Invited

Gold Nanoparticle Inside Graphene Shells: Prospects in Sensors and Plasmonics: *Nitin Chopra*[1]; [1]The University of Alabama

In–situ growth of graphene on noble metal surfaces is of great importance for applications in chemical and biological sensors and nanophotonics. In this talk, I will be discussing some major advancement made by us in the area of chemical vapor deposition (CVD) growth of graphene shells encapsulated gold nanoparticles (GNPs). This approach utilizes surface oxidized gold nanoparticles for the direct growth of well-controlled graphene shells around it. The growth approach also overcomes the issue of aggregation of nanoparticles during the CVD growth process and allows for the formation of stable dispersion of GNPs. A detailed analysis of morphological evolution and electron/analytical characterization of GNPs will be explained. As a next step, complex architectures of these hybrid nanoparticles are achieved on 1-D nanostructures such as CNTs and semiconducting nanowires. Mathematical modeling of plasmonic behavior, their biofunctionalization, and applications in sensors will be discussed.

11:10 AM

Carbon Nanotube Coated Conductor Composites: *Terry Holesinger*[1]; Raymond Depaula[1]; John Rowley[1]; Pallas Papin[1]; [1]Los Alamos National Laboratory

The development of industrially-scalable processes for aligning very thick coatings of carbon nanotubes (CNTs) on a suitable wire former is a key step in multi-functional CNT coated conductors. Aligned CNT coatings up to 100 microns thick have been prepared by conventional solution coating and wire drawing. We have successfully produced wires that display some of the lowest reported resistivity values for CNT coatings. For our best result, an overall wire resistivity was measured to be 2.12 ??-cm from which the CNT coating resistivity was calculated to be 5.5 ??-cm. In terms of conductivity, the composite wire and CNT coating values were 46 and 18 MS/m, respectively. Electron microscopy has been extensively used to identify and eliminate current limiting defects. Prospects for scale-up and application development will be discussed.This work was supported by the Research Partnership to Secure Energy for America (RPSEA) via subcontract 09121-3300-10 and the Chevron Corporation.

11:30 AM

Optical, Electrical and Electronic Properties of Vanadium Oxides – An Analysis: *Chiranjivi Lamsal*[1]; Nuggehalli Ravindra[1]; [1]New Jersey Institute of Technology

An overview of the optical, electrical and electronic properties of vanadium oxides, VO_2, V_2O_3, and V_2O_5, is presented. The properties are analyzed for various structures, as a function of polarization and temperature, utilizing phenomenological approaches. The first order reversible, insulator to metal (IMT) phase transition of the V-O systems is studied as an effect of temperature change. Electrical and optical conduction mechanisms are interpreted for both metal and insulating states using suitable models. Electronic properties are studied using electronic structure calculation packages.

11:50 AM

Encapsulating Polymeric Nitrogen in Carbon Nanotubes: *El Mostafa Benchafia*[1]; Zafar Iqbal[1]; Nuggehalli Ravindra; [1]New Jersey Institute of Technology

Polymeric phases of compounds, generally known only in their molecular forms, have been synthesized in minor quantities using High Pressure/Temperature approaches. Here, we present Plasma Enhanced Chemical Vapor Deposition as an alternative to synthesize a polymeric Phase of Nitrogen that can hold at ambient conditions using Carbon Nanotubes as substrate . This long sought-after polymeric Nitrogen is promising to be the highest density energetic material. Simplicity, ease and stability at ambient conditions make our approach very important. FTIR and Raman spectra along with DFT calculations are used to identify the structure and the vibrational frequencies assignment for this polymeric phase.
