2008 Nanomaterials: Fabrication, Properties, and Applications: Poster Session

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee
Program Organizers: Wonbong Choi, Florida International University; Seong Jin Koh, University of Texas at Arlington; Donna Senft, US Air Force; Ganapathiraman Ramanath, Rensselaer Polytechnic Institute; Seung Kang, Qualcomm Inc

Sunday, 6:00-8:00 PM Room: 273
March 9, 2008 Location: Ernest Morial Convention Center

Aluminum Alloy Based Nanocomposites Reinforced with Carbon Nanotubes: *Hyun-joo Choi*[1]; Donghyun Bae[1]; [1]Yonsei University

Aluminum alloy based nanocomposites reinforced with carbon nanotubes exhibiting high specific strength and toughness are produced by hot rolling of the ball-milled mixture of aluminum alloy powders and MWNTs (Multi-walled carbon nanotubes). Each of MWNTs is well dispersed during the milling and uniaxially aligned along the rolling direction. Especially, the tubes are found to be gradually filled with aluminum atoms as the milling time increases, providing the perfectly sticking interface between the MWNTs and the matrix. The strength of the composites increase with an increase of volume fraction of MWNTs up to 0.03, and the tendency is well matched with the conventional rule of mixture. Finally, the composite sheets containing 3 vol.% MWNTs with an area above 10 inch2 exhibit remarkably enhanced strength around 750MPa in tension tests. The details of reinforcing effects of nano-scale tubes including strengthening and toughening mechanism of the MWNTs will be presented.

Composition Evolution during FePt Nanoparticle Synthesis: *Chandan Srivastava*[1]; Jayendra Balasubramanian[1]; Gregory Thompson[1]; Christoffer Turner[1]; John Wiest[1]; [1]University of Alabama

FePt nanoparticles are candidate materials for future magnetic storage devices. Variation in composition and size from particle-to-particle is one of the factors limiting their application. In the present study, FePt nanoparticles were synthesized by two different synthetic routes: the iron pentacarbonyl route (involving the co-reduction of Fe and Pt precursors) and the superhydride route (involving a two step reduction of precursors). The mechanism of formation of particles was investigated by structural and compositional characterization of the reaction mixture, extracted at different stages of the synthesis. It was observed that the superhydride route produced particles with a narrower composition and size distribution than iron pentacarbonyl route. These differences will be discussed as a function of the evolution of composition during the synthesis. A Monte Carlo simulation has been performed supporting the mechanism theory and suggesting a thermodynamic limit for the incorporation of Fe into the core of FePt nanoparticles.

Dislocation Interactions with Σ11 Tilt Boundaries: *Joshua Askin*[1]; Richard Hoagland[2]; Peter Anderson[1]; [1]Ohio State University; [2]Los Alamos National Laboratory

Grain boundaries play a critical role in plasticity in nanocrystalline metals, where they act as both sources and sinks of dislocation content. A single set of grain misorientations can create a multitude of grain boundary structures, depending on the orientation of the grain boundary and rigid body translation of the two grains parallel to the grain boundary. Here we compare the interaction of several grain boundaries in the Σ11 tilt orientation with dislocations of differing Burgers vectors. Absorption is a common result, with the perfect dislocation dissociating into grain boundary dislocations or otherwise spreading its core on the grain boundary, lowering total system energy. The details of absorption vary both between boundaries and within a single boundary, as the local atomic configuration changes. Results from atomistic studies are viewed in the context of the gamma surface for the boundary and compared with Peierls-type continuum models of core spreading.

Effect of Nb and Sn on the Transformation of Alpha to Beta Titanium in Ti-35 Nb-2.5 Sn Alloy Using Mechanical Alloying: Abdel-Nasser Omran[1]; *K. Woo*[1]; D. Kim[1]; Sug Won Kim[1]; [1]Chonbuk National University, Divisions of Advanced Materials Engineering, Research Center of Industrial Technology

Titanium and its alloys have many uses in different medical fields. In titanium alloys, the principal effect of an alloying element is its effect on the alpha-to-beta transformation temperature. In this work, the niobium has been chosen as β stabilizer, and tin as reducer of elastic modulus. The starting materials were blended and milled using mixing machine (24hr) and high energy ball mill machine (1, 4, and 12 hr respectively). The particles size and phases of the produced powders were analyzed using XRD, SEM, TEM, and PSA. It was found that, the titanium was completely transformed from α to β Ti at milling time 12hr.

Electrical and Optical Properties of ZnO and Gallium Doped ZnO Thin Films Prepared by rf Magnetron Sputtering: Effect of Annealing and UV Radiation: *Ved Verma*[1]; Hoonha Jeon[2]; Minhyon Jeon[2]; Wonbong Choi[1]; [1]Florida International University; [2]Inje University

Zinc oxide (ZnO) and Ga doped (1wt%) zinc oxide (GZO) thin films are grown on SiO_2/Si and glass substrates at room temperature by rf magnetron sputtering. The structural properties of both ZnO and GZO thin films are investigated by high resolution x-ray diffraction and atomic force microscopy. Both the ZnO and GZO films grow in preferred orientation of <001> direction. However, GZO thin film shows higher surface roughness (rms~1.65 nm) than ZnO thin film (rms~1.0 nm). Electrical and optical properties of thin films are investigated by Hall Effect and UV-VIS-NIR spectrometer. Both the thin films show a transmittance, above 80%. The GZO thin films exhibit higher conductivity compared to that of ZnO thin films. With time, ZnO thin films show decrease in conductivity where as GZO thin films demonstrate a stable value, which can be attributed to the passivation of oxygen dangling bond by Ga atoms in GZO thin film.

Forming Surface Nanofilms on Particles of Dispersion Aluminium: *Sergey Lipko*[1]; Vladimir Tauson[2]; Boris Zelberg[1]; [1]Siberian Research and Design Institute for Aluminium and Electrode Industry JSC; [2]Institute of Geochemistry, SD, RAS

It is considered the influence of various chemical components on powder aluminium composition, produced using the method of gas dispersion of aluminium melt in nitrogen atmosphere and then annealed in different conditions. Powders with particles of different size 5-7 and about 20 mkm were examined. The presence of W makes better the structure of a film and promotes the formation of less strained nitride coating that was seen during comparative analysis of RFES width, pick no. 1s at half of maximum height after aluminium powder annealing in the presence of W in a sealed test-tube with air. It is anticipated that W has catalytic effect promoting the formation of nitric radicals that interact with particles' surface. W belongs to the group of elements with effect of integral accumulation in fine fractions of spray like Zn, Zr and some others (V.V. Skitina and others – DAN, 2003, v.390, no. 4, p.495-498).

Nano-Diamond Coatings for Machining Applications: *Jianwen Hu*[1]; Kevin Chou[1]; Raymond Thompson[2]; [1]University of Alabama; [2]Vista Engineering

Different from microcrystalline diamond (MCD) coatings, nanostructured diamond (nano-diamond) coatings, produced by microwave plasma-assisted chemical vapor deposition with nitrogen gas added, own several unique properties that enhance their machining performance in cutting tool applications. Characterized by nanoindentation, nano-diamond coatings have very high hardness (over 80 GPa vs. ~60 GPa of MCD) and lower elasticity (below 800 GPa vs. ~1100 GPa of MCD) which generates less residual stresses in the coating-substrate system. Moreover, nano-diamond coatings have much smoother topography than MCD coatings. Nano-diamond coatings consist of nanocrystalline diamond grains (average sizes from 5 to 30 nm) imbedded into an amorphous tetrahedral carbon matrix which offers cracking resistance. These distinct attributes jointly result in strong adhesion of nano-diamond coatings. Machining of high-strength Al alloys and composites using diamond tooling shows that nano-diamond coated tools significantly outperform conventional MCD tools, though both of them exhibiting delamination as the major tool failure mode.

Nanowires of AlN and Si_3N_4 Prepared from Amorphous Powders: Zhao Han[1]; Mei Yang[1]; Mingli Lv[1]; *Hongmin Zhu*[1]; [1]Beijing University of Science and Technology

Aluminum nitride and silicon nitride nano-powders were synthesized through a chemical reduction, of $AlCl_3$ and $SiCl_4$ by sodium in liquid ammonia. The product powders were amorphous and spherical agglutinating particles ranging from 1 to 10 nanometers in diameter. Single-crystalline aluminum nitride (AlN) and silicon nitride (Si_3N_4) nanowires with hexagonal structure were prepared by heating the amorphous nano-powders at 1300°C through 1450°C. The products obtained were characterized by X-ray diffraction(XRD), scanning electron microscopy(SEM), transmission electron microscopy(TEM), and selected area electron diffraction(SAED). The results revealed that the products were single-crystalline AlN and Si_3N_4 nanowires. The diameters of the nanowires ranged from 30 to 200 nm, and the lengths were from several micrometers to several decades of micrometers.

Novel Preparation and Characterization of Rare-Earth Nanoparticles and Nanocrystalline Bulks: *Xiaoyan Song*[1]; Jiuxing Zhang[1]; Nianduan Lu[1]; Markus Rettenmayr[2]; [1]Beijing University of Technology; [2]Friedrich-Schiller-Universität Jena

With a home-developed "oxygen-free" in-situ synthesis system, we produced a series of rare-earth nanoparticles with controllable size. In particular, we proposed an innovative route of preparing ultrafine nanocrystalline bulks with the sequentially performed processes: the amorphization of nanoparticles, nucleation and growth of the short-range ordered "clusters", and the complete nanocrystallization. By these procedures, the grain sizes in the resultant nanocrystalline bulks are much smaller than the initial nanoparticle sizes, representing the advantage of the present technique over the conventional power metallurgy methods. The microstructures and properties of the prepared nano rare-earths have been characterized systematically. The physical, thermal and mechanical properties of the prepared nanostructured bulks are found to be improved remarkably as compared with the conventional polycrystalline bulks. The present preparation technique has potentially wide applications to a big variety of metal nanomaterials that are active in the air.

Photoactive C60 Bridged Tetrameric Osmium and Ruthenium γ-Cyclodextrin Assemblies: Assembly and Spectroscopy: *Muath Atmeh*[1]; [1]Dublin Institute of Technology

Cyclodextrins display a rich host-guest chemistry. A particularly attractive proposition is to combine the properties of CD with luminophores, which may act as reporters of binding or other interactions at the cyclodextrin cavity. Ruthenium and osmium polypyridyl complexes are particularly attractive reporters in this regard because of their visible emission, their useful redox properties. In this contribution, we exploit this ability to design a tetrameric metallocyclodextrins containing photoactive Ru(II) polypyridyl units covalently bonded to γ-CD. The supramolecular assembly consists of cyclodextrin to which two ruthenium (II) or osmium (II) polypyridyl have been covalently linked these CDs then self-assemble with a fullerene moiety in 2:1 ratio to produce the tetramer, Figure 1. Here we describe the synthesis and characterization of the complexes and in particular their spectroscopic electrochemical and photophysical properties. We describe evidence for photoinduced processes and discuss the possibility of electron and energy transfers in these novel supramolecular assemblies.

Preparation of Nanosized Zinc Ferrite Particles: *Qing-hua Tian*[1]; Xueyi Guo[1]; Huang Kai[1]; [1]Central South University

Based on the review of technical literatures, the co-precipitation-drying-thermal decomposition was determined for the preparation of nanosized zinc-ferrite. The ammonium bicarbonate was chosen as the co-precipitation agent, and the thermodynamic analyses were done for the solution system of Fe(III)-Zn(II)-NH3-CO32—H2O. The double-jet precipitation process was proposed based on the thermodynamic analyses results. Considering the heavy aggregation among nano-sized particles, the measures were adopteed by addition of dispersant in the process of co-precipitation and washing by organic solvent or azeotropic distillation. By TG-DTA analysis, the suitable thermol-decomposition temperature of the zinc ferrite precursor was determined at about 450°C. Kept at this temperature for 2 hours, the pure and well crystalized $ZnFe_2O_4$ was obtained. SEM Photos of the obtained powder shows that the particles are uniform in size distribution (20nm-50nm) with good dispersivity.

Processing and Characterization of Ti_2AlC/Nanocrystalline Mg Matrix Composites: *Shahram Amini*[1]; Michel Barsoum[1]; [1]Drexel University

The MAX phases - of which Ti_2AlC is a member - are layered machinable, hexagonal ternary carbides and nitrides. Due to their high c/a ratios, the MAX phases deform primarily by the formation of kink bands and consequently are members – together with Mg - of a much larger class of solids labeled kinking nonlinear elastic, KNE. Herein we report on the fabrication and characterization of Ti_2AlC/nanocrystalline Mg matrix composites fabricated by hot pressing and pressureless melt infiltration. Hot-pressing of 50 vol. % Mg and Ti_2AlC powders at 750°C for 1 h at ~ 45 MPa resulted in fully dense composites. More importantly, fully dense samples were also made by pressureless infiltration of molten Mg into porous preforms of Ti_2AlC under vacuum. The Mg matrix existed in the form of ~ 35 and 50 nm diameter nanoparticles in hot pressed and infiltrated composites.

Quantum Size Effect of Electron Density and Its Influence on Interlayer Relaxation of Ultra-Thin Metal Films: Fei Ma[1]; Shengli Ma[2]; Kewei Xu[2]; *Paul Chu*[1]; [1]City University of HongKong; [2]Xi'an Jiaotong University

Further minimization of electronic devices and microelectromechanical systems (MEMS) requires the feature sizes of relevant materials to be shrunk significantly. In such a case, boundary effects, such as interfaces and surfaces, become remarkable, especially in nanometer scale, which must affect their microstructures and properties. In this work, we have analyzed the distribution of electron charge density in Cu and Al ultra-thin films using free electron model. The results show that an electrostatic field may come into being due to quantum size effect, and the interlayer separations must relax to decrease the Coulomb energy, the thinner the films, the larger the relaxation. More interestingly, the different electron shell configurations result in two opposite deviating directions of the center of negative charges: inwards for Cu and outwards for Al, and thus two absolutely distinct interlayer relaxations.

Robust and High Current Cold Electron Source Based on Carbon Nanotube Field Emitters and Electron Multiplier Microchannel Plate: *Raghunandan Seelaboyina*[1]; Srinivas Rao Bodepalli[1]; Wonbong Choi[1]; [1]Florida International University

Vacuum microelectronics has been studied for decades to develop unique devices such as rf-generators, high efficiency flat panel displays, x-ray sources and so on. In recent years field emitters based on carbon nanotubes (CNTs) and other nano materials have demonstrated high emission current densities making them prime candidates for next generation vacuum microelectronic applications. However the emission efficiency and stability of these materials is hindered by non uniform emission and emitter destruction in high electric field conditions. To achieve higher and stable current we have designed and fabricated a unique ceramic microchannel plate (MCP) consisting of high secondary emission yield (SEY) materials. The MCP was fabricated utilizing the optimum design parameters, which include channel dimensions and material properties obtained from charged particle optics (CPO) simulation. In this presentation we will discuss the results on our new microchannel plate design (simulation), fabrication, and field emission current amplification from vertically aligned carbon nanotube tower structures and microchannel plate assembly.

Size Dependent Elasticity of Nanowires: *Moneesh Upmanyu*[1]; [1]Colorado School of Mines

We employ a molecular statics approach based on embedded-atom-method (EAM) inter-atomic potentials to study the elasticity of metallic nanowires. Self-consistent comparison with the bulk response in copper clearly shows that the overall nanowire elasticity is primarily due to non-linear response of the nanowire core. While the surface stress induced surface elasticity modifies the behavior for ultra-thin nanowires, their contribution is always considerably smaller than that due to non-linear elasticity of the nanowire core. More importantly, for all three orientations, the surface is softer than an equivalently strained bulk, and the overall nanowire softening or stiffening is determined by orientation dependent core elasticity. Implications for heterostructured nanowires and nanotube bundles will be also discussed.

Structural Identification of Nanocrystals from High Resolution Transmission Electron Microscopy Images: *Peter Moeck*[1]; [1]Portland State University

A novel method for the structurally identification of nanocrystals from high resolution transmission electron microscopy images is described. Components of this method are demonstrated on both experimental and simulated images. There are several levels to this structural fingerprinting method that allow for increasingly discriminatory identifications of crystal structures out of a range of candidate structures from a database. With increasing identification power, these levels are extracting the projected reciprocal lattice geometry, plane symmetry group, structure factor amplitudes, and structure factor phases. If necessary for even higher levels of structural discrimination, the extracted structural information can be extended by direct methods and the errors that have been made by assuming kinematical scattering can be estimated and corrected for. The mainly inorganic subset of the Crystallography Open Database (http://nanocrystallography.research.pdx.edu/CIF-searchable/cod.php, with approximately 10,000 structure entries) and the Nano-Crystallography Database (http://nanocrystallography.research.pdx.edu/CIF-searchable/ncd.php) can be employed to facilitate the structural identification by calculating lattice-fringe fingerprint plots.

Study on Nano-Alumina Prepared by Low-Temperature Combustion Synthesis: *Guo Rui*[1]; [1]Northeastern University

Al_2O_3 has fine physical and chemical properties. Nanometer α-Al_2O_3 powder was prepared by the method of Low-temperature Combustion Synthesis with aluminum nitrate Nona hydrate and urea as raw materials in the muffle furnace and microwave oven. By the means of XRD, TEM, TG-DTA, IR and Malvern Mastersizer measurements, the as-prepared powder was analyzed. The optimum technology process with muffle furnace was: the molar ratio of Al(NO3)3•9H2O/CO(NH2)2 was 1 to 2.5,the igniting temperature was 750°C. It was found that the a-Al_2O3 powders having an average gain size about 40-90nm were sheet structure in a great measure, others were the shape of approximate sphere. The optimum technology process with the microwave oven was: the molar ratio of Al(NO3)3•9H2O/CO(NH2)2 was 1 to 2.5; heat power was 900W. The product having an average gain size about 60-90nm was sheet in a grate measure.

Synthesis and Characterization of Nano-Spinel Lithium Manganate: *Xinghua Xie*[1]; Shilong Yan[1]; Hongbo Wu[1]; Weiguo Wang[1]; Meng Wang[1]; Xiaojie Li[2]; [1]Anhui University of Science and Technology; [2]Dalian University of Technology

The formation of metallic nanooxides via detonation reaction was investigated with respect to the presence of an energetic precursor, such as the metallic nitrate and the degree of confinement of the explosive charge. The detonation products were characterized by scanning electron microscopy. The thermal stability of the nanostructures has been examined by heating-treatment at different temperatures. Powder X-ray diffraction, transmission electron microscopy, scanning electron microscopy, thermogravimetric analysis and BET were used to characterize the products. Nano-metallic oxides with diameters from 10 to 50 nm and a variety of morphologies were found. The oxides produced by this cheap method affirmed the validity of detonation synthesis of nano-size powders.

Synthesis and Electrical Properties of Exotic Boron Carbide Nanowires: *Varun Gupta*[1]; Steve Miller[1]; Giovanni Fanchini[1]; Jafar Al-Sharab[1]; Manish Chhowalla[1]; [1]Rutgers University

Recently, synthesis of one dimensional nano-materials and quasi-one dimensional nanostructures such as nanotubes, nanopipes and nanowires (NWs) has gained a large impetus. Boron carbide NWs are particularly significant because of their use in thermoelectric devices and other electronic applications. In this study we explore the role of boron/carbon ratio, temperature, inert gas pressure and dopants (Si and Al) on the morphology, length and diameter of nanowires. Nanowire dimensions show a bimodal distribution with wire length varying from 100nm to 50µm and up to a few millimeters. The elemental composition, morphology and single crystalline nature of the nanowires were analyzed by SEM, EDS, TGA and HRTEM. The effect of Si and Al doping on the conductivity is further evaluated and compared to pure B_4C. This approach can be readily extended to the synthesis of other doped nanostructures, which can offer great opportunities for both fundamental research and technological applications.

Temperature, Thickness and High Energy Si Ions Bombardment Effects on the Thermoelectric Properties of $GdFe_4Sb_{6-y}Ge_y$ Thin Films: *Sadik Guner*[1]; Satilmis Budak[1]; Claudiu Muntele[1]; Daryush Ila[1]; [1]Alabama A&M University, Department of Physics, Center for Irradiation of Materials

We have grown three monolayer $GdFe_4Sb_{6-y}Ge_y$ (y = 2,4) thin films on silica substrates with varying thickness between 100-1000 nm using electron beam deposition. The high-energy (MeV) Si ion bombardments were performed on samples with varying fluencies ($1x10^{14}$-$5x10^{15}$). The thermopower, electrical and thermal conductivity measurements were carried out before and after the bombardment on samples to determine the dimensionless figure of merit, ZT. The Si ions bombardment caused changes on the thermoelectric properties of films. The fluence and temperature dependence of cross plane thermoelectric parameters were also reported. Rutherford Backscattering Spectrometry (RBS) was used to analyze the elemental composition of deposited materials and to determine the layer thickness of each film. Research sponsored by the Center for Irradiation of Materials, Alabama A&M University and by the AAMURI Center for Advanced Propulsion Materials under the contract number NNM06AA12A from NASA, and by National Science Foundation under Grant No. EPS-0447675.

The Anodic and Cathodic Processes in Direct Electrochemical Conversion of Solid Metal Chlorides to Metal Nanoparticles in Ionic Liquids: Linpo Yu[1]; Huijiao Sun[1]; Dihua Wang[1]; Xianbo Jin[1]; *George Chen*[2]; [1]Wuhan University; [2]University of Nottingham and Wuhan University

Solid metal chlorides have been attached to a metallic substrate in the form of either a thin coating or powder and successfully electrochemically reduced to metal nanoparticles in an ionic liquid, 1-butyl-3-methylimidazolium hexafluorophosphate. Particularly, the presentation compares the cyclic voltammograms of cuprous copper in aqueous and ionic liquid electrolyte, and the physicochemical characterisations of the potentiostatic electrolysis products on both cathode and anode. Preliminary findings are also presented for a few other metal chlorides. It is proposed that the formation of the metal nanoparticles is the result of a combined effect of the slow kinetics of the dissolution-deposition process in the ionic liquids, and also likely the ionic liquid being effective in preventing the metal particles to grow larger as compared with water.

The Fabrication Technique for Indium Tin Oxide Nanosized Composite Powder: *Huimin Lu*[1]; Xi Zhang[1]; [1]Beijing University of Aeronautics and Astronautics

Indium tin oxide (ITO) nanosized composite powder not only can improve sintering properties of target and afford material for big size and super density ITO target, but also can be made into electronic pastes which can be spurted on cathode ray tube as an effective seclusion screen of electromagnetic interfere. In this paper, conductive indium tin oxide(ITO) powder sin size of nanometer were prepared by the hydrolysis of corresponding metal salts following co-precipitation technique using indium metal ingots and SnCl4•5H2O as raw materials. On the purpose of manufacturing functional powders in a large amount and energy-conserving, the factors in whole course were considered, especially the influences of co-precipitation terminal pH value and heat treatment temperature under hydrogen gas on the particle size and power resistance were discussed. The characteristics of powers were investigated by DTA-TG, XRD, TEM.

The Influence of Nano Boehmite on Spinel Formation: *Hamid Zargar*[1]; Farhad Golestani Fard[1]; Hamidreza Rezaie[1]; [1]Iran University of Science and Technology

The effect of nano boehmite as an additive on the formation of spinel at low temperatures (T<1000°C) via solid-state procedure is investigated. In this regard, the homogeneity of prepared mixtures preciously studied by performing XRD, FTIR, SEM and MAP. Furthermore, in order to evaluate the morphology of synthesized spinel, SEM has applied. Results are implied that nano boehmite facilitate solid-state spinel formation on magnesia grain at temperatures as low as 700°C. In addition, prepared spinel is in nano scale (<80nm) and homogeniously distributed on, magnesia grains.

Thermoelectric Generator from Sequentially Deposited $SiO_2/GdFe_4Sb_{6-y}Ge_y$ Nanolayers Modified by MeV Si Ions Bombardment: *Sadik Guner*[1]; Satilmis Budak[2]; Claudiu Muntele[2]; Daryush Ila[2]; [1]Alabama A&M University, Department of Physics, Center for Irradiation of Materials; Fatih University, Department of Physics; [2]Alabama A&M University, Department of Physics, Center for Irradiation of Materials

We have grown 50-100 periodic nano-layers of $SiO_2/GdFe_4Sb_{6-y}Ge_y$ super-lattice electro-cooling system. The deposited multi-layer films have a periodic structure consisting of alternating layers, between 5-20 nm thick each. The super-lattices were then bombarded by 5 MeV Si ions at different fluences ranging from $1x10^{14}$ to $5x10^{15}$ ions/cm^2 to form nano-cluster structure. Rutherford Backscattering Spectrometry (RBS) specified the total deposit thickness and stoichiometry. We measured the thermoelectric efficiency of the fabricated device before and after MeV bombardments. To accomplish this we measured the cross plane thermal conductivity by 3rd harmonic method, cross plane Seebeck coefficient and cross plane electric conductivity. As predicted the electronic energy deposited due to ionization by MeV Si beam in its track produces nano-scale structures that disrupt and confine phonon transmission therefore reducing thermal conductivity, increasing electron density of state so as to increase Seebeck coefficient and electric conductivity, thus increasing the figure of merit. Research sponsored by the Center for Irradiation of Materials, Alabama A&M University and by the AAMURI Center for Advanced Propulsion Materials under the contract number NNM06AA12A from NASA, and by National Science Foundation under Grant No. EPS-0447675.

Computational Thermodynamics and Kinetics: Poster Session

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, ASM Materials Science Critical Technology Sector, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee, TMS/ASM: Phase Transformations Committee
Program Organizers: Yunzhi Wang, Ohio State University; Long-Qing Chen, Pennsylvania State University; Jeffrey Hoyt, McMaster University; Yu Wang, Virginia Tech

Sunday, 6:00-8:00 PM Room: 288
March 9, 2008 Location: Ernest Morial Convention Center

Session Chairs: Yunzhi Wang, Ohio State University; Long Qing Chen, Pennsylvania State University; Jeffrey Hoyt, McMaster University; Yu Wang, Virginia Tech

Development and Calibration of Pseudo-Binary Phase Field Modeling for Microstructural Evolution in Multi-Component Alloys: *Billie Wang*[1]; James Lill[2]; Youhai Wen[3]; Jeff Simmons[4]; Yunzhi Wang[1]; [1]Ohio State University; [2]High Performance Technologies Inc.; [3]UES Inc.; [4]Air Force Research Laboratory

Alloy development time is under constant pressure to be reduced. Physics-based modeling promises to make the most efficient use of experimentalist time by identifying processing windows for the formation of desirable microstructures. In order to be incorporated into the development cycle, a model must be calibrated rapidly and accurately, and be computationally efficient. To this end, a pseudo-binary phase field methodology that captures the kinetics of microstructural evolution of a multi-component system was developed. The parameters for the pseudo-binary model were optimized using the simplex method to match experimental measurement on average particle size as function of time. A penalty function was defined to quantify deviation from target parameters and accounts for uncertainty in literature, database and experimental data. Preliminary results will be presented.

First Principle Calculation of the Structural and Electronic Property of Zr Doped $B_{13}C_2$: *Yu Liang*[1]; Ru Hongqiang[1]; Jiang Yanli[1]; Zuo Liang[1]; Xue Xiangxin[1]; [1]Northeastern University

The first principle calculations based on density functional theory were carried out to study the stability and electronic properties of three structural unit models of Zr atom doped boron carbides ($B_{13}C_2$) crystal using CASTEP code which employed a plane wave-pseudo potential expansion technology. The calculations results show that Zr atom doped boron carbide is in preference to substituting C atom on the end of boron carbide chain, a representative structural unit containing Zr atom is [C-B-Zr] ε+-[B11C] ε-,while the structural unit without Zr is [C-B-C] ε—[B11C] ε+, The band and density of states(DOS) indicates that the coexistence of these two different structural units makes the electrical conductivity increased. As the covalent bond of Zr-B is weaker than those of B-B and B-C, and the thermal conductivity decreases when Zr doped $B_{13}C_2$, the thermoelectric property of Zr doped boron carbides will be improved.

Grain Growth Simulations with Langevin Noise: *Nele Moelans*[1]; Frans Spaepen[2]; [1]Katholieke Universiteit Leuven; [2]Harvard University

We have added, in a thermodynamically consistent way, Langevin noise to a diffuse interface (phase field) model for grain growth. With this model we simulated how thermal noise affects grain growth. The total energy content of the simulated system was measured as a function of time. Energy jumps were linked to special events in the grain growth process, for example the disappearance of a grain. Depending on the magnitude of the noise, certain events and processes are induced or accelerated. Furthermore, we studied the stability and occurrence of (local) metastable grain configurations as a function of the magnitude of the noise. Langevin noise is also successful in preventing artificial pinning and drag in simulations, for example as a result of low resolution of the numerical technique.

Investigation of Atom Size Effects on Binary Alloys Phase Diagrams Using a Relaxed Monte Carlo Approach: *Mathieu Fevre*[1]; Alphonse Finel[1]; Yann Le Bouar[2]; [1]ONERA; [2]CNRS-ONERA

The precise determination of phase diagrams is essential to understand the microstructural evolution in metallic alloys. Theoretical predictions are difficult and usually rely on simplifying assumptions, such as interatomic potentials on a rigid lattice. In this study, we investigate a more realistic situation where atoms can move freely and interact through a position dependent potential. Using relaxed Monte Carlo simulations, we calculate the phase diagram of binary alloys exhibiting a phase separation (Cu-Ag type) or an order-disorder transformation (Cu-Au type). The whole composition range, from low temperature up to the liquid state is considered. By changing the parameters values of the potential, we have systematically studied the evolution of the phase diagram when the difference between the atomic radii of the two components is increased. The understanding of the phase stability in thin films and nanoparticles, where elastic relaxations play a major role is a natural extension of this work.

Kinetic Study on Chromium Ore Dissolution in $CaO-SiO_2-MgO-Al_2O_3$ Melts: Jiang Maofa[1]; Yan Liu[2]; De-yong Wang[1]; Li-xian Xu[1]; *Haiyan Zheng*[3]; [1]School of Materials and Metallurgy of Northeastern University; [2]Research Center for the Science and Technology of Shenyang University; [3]Institute of Ferrous Metallurgy of Northeastern University

To reveal the smelting reduction mechanism of chromium ore for producing stainless steel in converter, the dissolution behavior of chromium ore in CaO-SiO_2-MgO-Al2O_3 slag system was studied by laboratory experiments, and the effect of different temperature and slag composition on the dissolution rate of chromium ore in slag was investigated. The dissolution mechanism of chromium ore in slag was discussed. A kinetic model for dissolution process of chromium ore was developed on macrokinetics theory for the first time. According to the data of dissolution experiments, the regression expression between the dissolution rate constant and the temperature and slag composition was obtained. It was found that the dissolution process of chromium ore is controlled by the surface dissolution reaction on conditions of the present experiments, where the temperature has significant effect on the reaction rate constant of chromium ore dissolution. The calculated value of dissolution activation energy is 524.50kJ·mol-1.

Model Study and Forecast on the Behavior of Rare Earth during Solidification Process of Heavy Rail Steel: Liu Chengjun[1]; Fang Lei[1]; *Jiang Maofa*[1]; Haiyan Zheng[1]; [1]Northeastern University

A thermodynamic model was developed to describe quantificationally elements segregation and inclusions precipitation during solidification process of heavy rail steel. According to the SEM and energy spectrum analysis, the model could completely consist with experimental results. The state of RE and constituents of inclusions in heavy rail steel with different cleanliness were studied. The results

as follows: (1) The increment of RE dissolved in heavy rail steel mainly has two stages: the first stage is before the RE second phases were not precipitated, the second stage is after the separation react of the RE second phases reached equilibrium. And the increment of the second stage is more obvious. (2) Under the conditions of the same RE addition, the content of solid lanthanum dissolved in heavy rail steel is more than that of cerium. Alloying function of lanthanum is better than that of cerium.

Modeling of Oxygen Kinetics in a Ag/MgO Composite: *Nilindu Muthubandara*[1]; Irina Belova[1]; Andreas Oechsner[2]; Graeme Murch[1]; [1]University of Newcastle; [2]Technical University of Malaysia

The presence of atomic oxygen at metal/oxide interfaces can significantly affect the physical properties of interfaces and hence the properties of the bulk material. We modeled oxygen diffusion in Ag-MgO composites with a Lattice Monte Carlo method and the finite element method. First, we considered oxygen in-diffusion from a constant surface source solely into a Ag metal matrix: oxygen depth profiles were in excellent agreement with exact results. Next, we simulated oxygen in-diffusion/segregation in the composite permitting and restricting the mobility of oxygen in different scenarios involving the Ag-MgO interface. The (higher temperature) out-diffusion of oxygen from the composite was also simulated and corresponding results obtained for the oxygen depth profiles. In both cases, very good agreement was found between the Lattice Monte Carlo method and the finite element method.

Numerical Simulation of Twin-Roll Strip Casting Process: Jieyu Zhang[1]; *Bo Wang*[2]; [1]Shanghai University; [2]Inner Mongolia University of Science and Technology

A three-dimensional mathematical model has been developed to simulate fluid flow, heat transfer, and solidification in twin-roll strip casting of steel. The two equation model is used to incorporate the turbulence in fluid flow. The effect of the casting speed, superheat, and roll gap on the flow and temperature field was predicted. The simulation results showed that it was desirable for the wedge metal delivery system to not only gain the uniform of flow and temperature in the pool, but also improve strip quality and ensure casing process.

Phase Field Study of Precipitate Growth Kinetics: Effect of a Misfit Strain: Rajdip Mukherjee[1]; Thennathur Abinandanan[1]; *Mogadalai Gururajan*[2]; [1]Indian Institute of Science; [2]Northwest University

Laraia and Johnson presented a model for the kinetics of growth of an isolated, dilatationally misfitting precipitate. Our study - using a phase field model based on the Cahn-Hilliard equation - is aimed at validating their results through 'computer experiments', since those results are not amenable for direct experimental verification. We first establish the validity of phase field experiments by showing that the parabolic growth coefficient obtained from our phase field simulations is in very good agreement with that obtained through a numerical solution of the classical Zener problem with a variable diffusivity. We then show that the parabolic growth coefficient for a dilatationally misfitting precipitate is in agreement with that obtained from the sharp interface model (modified to account for composition-dependent diffusivity) of Laraia and Johnson. In more supersaturated alloys, since curvature effects are smaller, the agreement between phase field results and those from the sharp-interface model is better.

Thermodynamics of Liquid Phase Sintering of SiC Using Al_2O_3 and Y_2O_3 as Sintering Additives: *Hans Seifert*[1]; Damian Cupid[2]; Olga Fabrichnaya[1]; [1]Technische University Bergakademie; [2]University of Florida

A thermodynamic dataset for the Al–C–O–Si–Y system was used for calculations of multicomponent, multiphase reactions. Some aspects of the liquid phase sintering of silicon carbide using alumina and yttria sintering additives were analyzed. The phase relations in the SiC–Al_2O_3, SiC–Al_2O_3–SiO_2 and SiC-Y_2O_3–SiO_2 systems were calculated. Phase fraction diagrams, isopleths, isothermal sections, and potential phase diagrams are presented to illustrate the reactions between silicon carbide and sintering additives. The effect of Ar inert gas as an additional component and the related volume change of the gas phase were considered. In addition, the influence of surface silica on silicon carbide powder is taken into account.

General Poster Session

Sponsored by: The Minerals, Metals and Materials Society

Sunday, 6:00-8:00 PM
March 9, 2008

Room: Hall I-2
Location: Ernest Morial Convention Center

Application of Amide–Impregnated Fiber to Separation of Precious Metals: *Hirokazu Narita*[1]; Mikiya Tanaka[1]; Kazuko Morisaku[1]; Ken Tamura[2]; Daisuke Sakamoto[3]; Masashi Suzuki[3]; Tomomi Nadano[3]; [1]National Institute of Advanced Industrial Science and Technology; [2]Chiba Institute of Technology; [3]Saitama Industrial Technology Center

The separation of precious metals in a hydrochloric acid solution using a solvent impregnated fiber (SIF) was investigated. N-disubstituted amide compounds and kapok fibers were used as the separation reagents and the impregnation support, respectively. We synthesized N,N-di-n-octyl-lauramide (DOLA), N,N'-dimethyl-N,N'-di-n-octyl-thiodiglycolamide (MOTDGA) and N,N'-dimethyl-N,N'-di-n-octyl-diglycolamide (MODGA) and prepared the amide-impregnated fibers (amide–IF). The adsorption of some precious and base metals (Au(III), Pd(II), Pt(IV), Rh(III), Fe(III), Cu(II), Ni(II) and Zn(II)) in HCl solutions was carried out batchwise using the DOLA–IF, MODGA–IF and MODGA–IF. The results of the metal adsorption showed that the selective separation of Au(III), Pd(II) and Pt(IV) can be performed using successively the DOLA–IF, MOTDGA–IF and MODGA–IF.

Changes in Hydrogen Permeability and Microstructure of Melt-Spun $Nb_{40}Ti_{30}Ni_{30}$ Alloy Ribbons by Annealed: *Yuta Seki*[1]; Koichi Kita[2]; Kazuhiro Ishikawa[1]; Kiyoshi Aoki[1]; [1]Kitami Institute of Technology; [2]Mitsubishi Materials Corporation

Pd-Ag based hydrogen permeation alloys are mainly used for separation and purification of hydrogen gas. However, since Pd is too expensive and a rare metal, it is strongly desired to develop non-Pd based alloys. The Nb-TiNi alloys consisting of the bcc-(Nb, Ti) and the B2-TiNi phase show high hydrogen permeability equivalent to that of pure Pd. However, its membrane is prepared by means of complex processes such as cold rolling and intermediate annealing. On the other hand, it is well known that alloy ribbons can at a stroke be obtained by a melt-spinning technique. In the present work, hydrogen permeability, crystal structures and microstructures of melt spun Nb-TiNi alloy ribbons before and after annealing treatments are investigated in order to develop the preparation method of alloy membrane, and it was concluded that melt-spinning technique is effective for the preparation of the Nb-TiNi hydrogen permeation alloy membrane.

Characterization and Research of Nano-Meter ZnO by X-Ray Diffraction: *Cheng Guofeng*[1]; [1]Shanghai Institute of Ceramics

The microstructures (average crystallite size and stacking faults probability) and the doped effects of the nano-meter ZnO have been characterized and researched using separating multip-broadening effects method improved by author. The results are following: (1) The crystallite size of studied two group samples are a few huandreds and several nano-meter respectively. The crystallite shape of the two groups ZnO samples nearly are the same polohedron,but the difference among them can be characterized by. (2) The method for separating two-fold and three-fold broadening effects of closed packing hexagonal is not used to the nano-meter ZnO samples, because the seletive broadening effects is also not obviously. (3) The selective broadening effects of stacking faults may be ignored, because the stacking faults probability of the two groups ZnO samples is very small.

Chemical Composition Effects on the Microstructure of Functionally-Graded Aluminum Matrix Composites: *Lilia Olaya-Luengas*[1]; Marcelo Suarez[1]; [1]University of Puerto Rico, Mayagüez

Aluminum matrix composites reinforced with boride dispersoids redefine the limits of aluminum-based materials due to their unique mechanical properties, low density and low-cost processing methods. In addition, by centrifugal casting a functionally-graded composite can be fabricated. The redistribution of the denser dispersoids in the aluminum matrix is further affected by changes in the levels of boron, magnesium, copper and calcium. The present research has

been focused on studying the functionalized composite microstructure and the resulting graded mechanical properties. The final goal has been to determine the optimal reinforcement distribution as a function of the chemical composition of the material.

Co-Doping (Ti3+, Fe3+, and Zr4+) in NaAlH4 Powders Studied by Ultra-Small-Angle X-Ray Scattering (USAXS): *Ejiroghene Oteri*[1]; Tabbetha Dobbins[1]; [1]Louisiana Tech University

This study uses ultrasmall angle x-ray scattering (USAXS) to elucidate differences in NaAlH4 particle morphology as dopant type and mill time is varied after co-doping using FeCl3-TiCl3, FeCl3-ZrCl4, and TiCl3-ZrCl4. In these co-doped systems, USAXS was used to track changes in powder surface area using measured particle sizes and volume fractions. The variation in desorption rates in those co-doped systems correlated well with changes in powder surface area—indicating surface reaction rates are the limiting factor in hydrogen desorption kinetics for these systems.

Comparison of the Atomic and Electronic Structure of Single F Centers in Cubic $PbZrO_3$, $PbTiO_3$, and $SrTiO_3$ Perovskites: *Yuri Zhukovskii*[1]; Sergei Piskunov[1]; Eugene Kotomin[1]; Donald Ellis[2]; [1]University of Latvia, Institute of Solid State Physics; [2]Northwestern University

Hybrid DFT-LCAO calculations were performed using 3×3×3 supercells of defective cubic perovskites. Outward displacements of Zr and Ti atoms nearest to oxygen vacancy (F center) are 1% ($PbZrO_3$) vs. 3% ($PbTiO_3$). Inward relaxation of next-nearest oxygens is larger in zirconate (10 vs. 2%), similarly to inward shift of following leads (12 vs. 5%). Strontium relaxation around F center is almost negligible. F center formation energy is larger in $SrTiO_3$ (8.75 eV) relatively to $PbZrO_3$ and $PbTiO_3$ (7.25 vs. 7.82 eV). O vacancies in $PbZrO_3$, $PbTiO_3$ and $SrTiO_3$ trap 0.7, 0.9, and 1.2 e. Band structures show different defect level location. For zirconate, it lies 1.72 eV below bottom of conduction band, with small dispersion over Brillouin zone (0.14 eV). For $PbTiO_3$ vs. $SrTiO_3$, this level is closer to CB, with larger dispersion (0.97, 0.21 vs. 0.69, 0.25 eV). Thus, different chemical nature of cations results in considerable variation of properties.

Deformation Behavior of Magnesium Alloys with the Low c/a Ratio: *Beomsoo Shin*[1]; Donghyun Bae[1]; [1]Yonsei University

Deformation behavior of Mg-Re-Zn-Sn alloy sheets has been investigated. The sheets are produced by the conventional thermomechanical processes. Tensile tests were performed at a strain rate of 1x10-3s-1 at room and elevated temperatures. The alloys exhibit superior tensile elongation higher than 25% at room temperature. The deformed microstructure shows that the contribution of deformation twinning to total elongation is not so significant, and non-basal dislocations are frequently observed. The non-basal slips can be activated not by the presence of refined grains, but by the low c/a ratio of alpha magnesium phase. The c/a ratio of the phase is measured to be below 1.6. The details of deformation behavior of the alloys will be presented.

Deformation Behavior of Zr-Based Bulk Metallic Glasses Showing No Catastrophic Failure at Room Temperature: *Jaehyuck Shin*[1]; Donghyun Bae[1]; [1]Yonsei University

Plastic deformation of bulk metallic glasses (BMGs) at room temperature occurs within the highly localized shear bands in which generated excess free volume is spontaneously coalesced, leading to a catastrophic failure of the BMGs even under compression. Therefore, to prevent the catastrophic failure, atomic clustering kinetics should be retarded. Zr-Al-Cu-Ni BMGs with high thermal activation energy have shown a highly deformable behavior without global failure under compression. In addition, further plastic homogeneity in the macroscopic appearance can be achieved with the addition of minor elements in the Zr-based BMGs due to the formation of abundant nano-scale ordered sites which initiate multiple shear bands. With the consideration of structural thermal stability, together with free volume, deformation behavior of Zr-based bulk metallic glasses which show no catastrophic failure at room temperature will be discussed.

Effect of Cr on the Oxidation Behavior of Ti-46Al-2V Alloy: *Daniela Pilone*[1]; Ferdinando Felli[1]; [1]Sapienza Università di Roma

Titanium aluminide alloys are already used because of excellent mechanical properties, but are limited to low temperature applications due to insufficient oxidation resistance. When these alloys are subjected to oxidation in air the scale is not a protective Al2O3 layer, but a mixture of Al2O3 and TiO2. The oxidation resistance of TiAl intermetallics is known to be significantly affected by the addition of alloying elements. The oxidation behavior of Ti-46Al-2V was studied and compared with the ones of the same alloy alloyed respectively with 7, 10 and 14 at.% Cr. Isothermal tests were conducted in air at 850 and 950°C. The scale's morphology and composition were studied by means of SEM/EDS and X-ray diffraction. From weight gain curves and cross-sectional microscopy after oxidation exposure it was found that more than 7 at.% of Cr improves the oxidation resistance of the alloy, although it simultaneously reduces its toughness.

Effect of Prior Deformation on the Sliding Wear Characteristics of the Ultra-Fine Grained (UFG) Dual Phase Steel: *Yong-suk Kim*[1]; H. Yu[1]; D. Shin[2]; [1]Kookmin University; [2]Hanyang University

Effect of prior deformation on the sliding wear of the ultra-fine grained (UFG) ferrite-martensite dual phase (DP) steel was investigated. The UFG DP steel was fabricated by the ECAP and subsequent intercritical annealing. The steel was cold rolled before the wear test, and the effect of the prior deformation on the wear was examined. The wear tests were carried out at various loads against a bearing steel ball. The wear rate of the UFG DP steel that did not experience the prior deformation was higher than that of the coarse-grained (CG) DP steel, because of more severe surface shear deformation. The wear rate of the specimens with prior deformation was much higher than that of the specimen without prior deformation. The deformed CG DP specimen showed higher rate than the deformed UFG DP specimen, and the rate-variation of the CG DP steel was much bigger under the same test condition.

Effects of Initial Texture on the Deformation Behaviors of Strip Cast AZ31 Mg Alloy: *Byoung Ho Lee*[1]; Sung Hyuk Park[1]; Chong Lee[1]; Wonkyu Bang[2]; Sangho Ahn[2]; [1]Pohang University of Science and Technology; [2]Research Institute of Industrial Science and Technology

The effect of initial texture on the deformation behavior of AZ31 Mg alloy was (manufactured by strip casting method) investigated in this work. XRD experiments showed that a strong basal texture (implying that the basal planes of HCP lattice in grains were located parallel to the rolling direction) was formed in the rolled plate, while a weak and random basal texture was formed in a strip cast sheet and cast ingots, respectively. Compressive specimens were obtained in two different directions, ND (normal direction) and RD (rolling direction). Microstructure observations and stress-strain curves showed that twin formation in strip-cast AZ31 Mg alloy was strongly affected by initial textures. Constitutive modeling of materials having different initial textures was also conducted in this work through physically-based modeling.

Elastic-Plastic Stress and Deformation Analysis of Annular Plates under Prescribed Radial Loading: *Ahmed Elkholy*[1]; Abdulazim Falah[1]; [1]Kuwait University

A modified from of constitutive equation for an isotropic elastic-plastic deformation of circular plates subjected to radial tensile loading on the inner surface is introduced. The form takes into consideration the effect of rotation of various principal axes and material hardening during the process of continued deformation. Plastic instability analysis of plates is carried out to determine stresses at the onset of cavity formation. Both symmetric and antisymmetric modes of deformation are determined. It was found out that the modified form which is derived in this study leads to deformation stresses which are lower than those obtained when classical plasticity relations are used, and therefore, are comparable with the results obtained experimentally. It is found also that deformation is asymmetric with respect to the plate axis and depends not only on the stress in the current state but also on the prescribed incremental traction ratio and material properties.

Hydrogen Permeability of Pure Nb and NbTi Solid Solution Alloys: *Naoyoshi Ota*[1]; Kazuhiro Ishikawa[1]; Kiyoshi Aoki[1]; [1]Kitami Institute of Technology

In recent years, non-palladium based hydrogen permeation alloys have actively been investigated by several research groups. Group 5 metals such as V, Nb and Ta showing large hydrogen solubility and high hydrogen diffusivity are promising for hydrogen permeation membranes, because hydrogen permeability is the product of hydrogen solubility and hydrogen diffusivity. However, it is recognized that these metals suffer severe hydrogen brittleness and are

pulverized spontaneously during hydrogenation. Then, they are unusable as a hydrogen permeation alloy. However, it is still uncertain why they are easily broken in a hydrogen atmosphere. In the present work, hydrogen permeability of as-cast pure Nb and the NbTi alloys prepared by arc melting were successfully measured using a conventional gas permeation method. We discuss why hydrogen permeability of the as-cast pure Nb and the NbTi alloys is measurable on the basis of the microstructural observation.

Inoculation of Aluminum Alloys with Nanosized Borides and Microstructure Analysis: *Hermes Calderón*[1]; Cicily Smith[2]; Olga Menéndez[1]; O. Marcelo Suárez[1]; [1]University of Puerto Rico; [2]Austing College

The effect of MgB_2, AlB_2, HfB_2, and NbB_2 nanosized particles on the grain structure and microhardness of AA6061 and AA7075 aluminum alloys was studied. The metal boride powders were processed with a vario-planetary ball milling unit to be afterwards mixed with pure aluminum pellets. The resulting mechanical mixture was added as inoculant to the aforementioned alloys. For comparison the alloys were separately treated with a commercial grain refiner. Changes in grain size were observed: while boride-treated AA7075 presented a dendritic structure, the boride-inoculated AA6061 alloy exhibited equiaxed grain structure. Vickers microhardness tests showed that MgB_2 and HfB_2 were most effective in improving mechanical strength of these aluminum alloys. Additionally, Charpy impact test were performed to identify the effect of inoculation on the treated alloys toughness.

Laser Synthesis of Porous and Textured Ca-P Bio-Ceramic Coating on Ti-6Al-4V: *Sameer Paital*[1]; Narendra Dahotre[1]; [1]University of Tennessee

In the present work the feasibility of depositing a porous and geometrically textured Calcium Phosphate (CaP) bio-ceramic coating using a continuous wave Nd:YAG laser on a Ti-6Al-4V substrate has been demonstrated. Advantages offered by such porous bio-ceramic coating is its inertness combined with the mechanical stability of the highly convoluted interface that develops when bone grows into the pores of ceramic. Non-destructive phase analysis of the laser processed samples were carried out using XRD. Quantitative estimation of the crystallite size and relative amounts of Ti, TiO2 and a-tricalcium phosphate (α-TCP) was obtained. Surface porosity measurements indicated a decreasing trend with increasing laser fluence. In the preliminary studies, the bioactivity of the coatings were further proved by the formation of an apatite like layer on the surface of the sample after being immersed in a simulated bio fluid.

Layer by Layer Nanoarchitectures Assembled Using Al2O3 and ZrO2 Systems: *Kristan Moore*[1]; Tabbetha Dobbins[2]; [1]Grambling State University; [2]Louisiana Technical University

For controlling the content and spatial distribution of interphase boundaries in materials, we have used a technique known as layer-by-layer (LbL) nanoassembly. The principle behind electrostatic self-assembly is the use of polyelectrolytes (for example, polyallylamine hydrochloride as polycation and polystyrene sulfonate as polyanion) to provide a coulombic 'glue' between ceramic particulate layers. The inherent surface charge (zeta-potential) on the particulate systems leads to their attraction to the polyelectrolytes. The self-assembly technique has been used to deposit multilayered ceramic films and also been used to provide nm-particle coverage over µm-scale colloidal particles. Using LbL nanoassemlby, we have prepared various Al2O3 and ZrO2. The concentration of the nanoparticles in suspension and deposition time was studied to affect the degree of microstructure control during self-assembly.

Mean Width Evaluation on Regular Grids: *Seth Wilson*[1]; A.D. Rollett[1]; [1]Carnegie Mellon University

We develop and compare several methods to compute the mean width (first-order Minkowski functional) of grains represented on regular grids. Error analysis is presented for a variety of shapes with cusps, creases, facets, and curved surfaces whose mean widths are known exactly. We use our mean width measurements to test the 3D generalization of the vonNeumann-Mullins relation conjectured by MacPherson and Srolovitz (Nature 2007), in the context of multi-phase field and Monte Carlo models of isotropic normal grain growth. Results are presented for single grains as well as large networks of grains.

Measuring Enhanced Elevated Temperature Deformation Using Spark Plasma Sintering Equipment: *Dustin Hulbert*[1]; Dongtao Jiang[1]; Amiya Mukherjee[1]; [1]University of California

A fully dense nanocrystalline ceramic consisting of ZrO2, Al2O3 and MgAl2O4 was deformed at 1150ºC at a strain rate on the order of 10-2 s-1. Spark plasma sintering was used in this study as a means of consolidation as well as for measuring elevated temperature deformation. By using the constitutive equation for elevated temperature plasticity in conjunction with previously measured strain rate sensitivities and activation energies a strain rate on the order of 10-6 s-1 is predicted at 1150ºC. This strain rate is four orders of magnitude slower than that measured using the spark plasma sintering equipment. This suggests some significant enhancement of the kinetics of deformation garnered by the pulsing electric field found inside the SPS chamber.

Metals Industry Air Metals Emissions and Hazard Rankings: *John Heinze*[1]; Karen Hagelstein[2]; [1]Environmental Health Research Foundation; [2]TIMES Limited

Total releases of metal air emissions (18 metals) from the metals manufacturing industry (SIC33XX) were over 3400 tons in 2005, according to the latest US EPA Toxic Release Inventory data. These emissions represent the largest source of metal air emissions of any industry sector in the US. Because metals have well recognized human health and the environmental hazard properties, metal air emissions can be prioritized not only by the amount of metal compounds released, but also by their hazard properties, also called "toxicity weighting." For example, the five most toxic metals according to EPA's Toxicity Characteristic Leaching Procedure (TCLP) for hazardous waste metal compounds are: mercury, followed by cadmium and selenium, and then arsenic and lead. The Indiana Relative Chemical Hazard Score (IRCHS) and other methods of hazard ranking will be evaluated and compared as methods for prioritizing hazard impacts and environmental management practices in metals manufacturing.

Microstructural Characterization in Cast AlMg Alloy-SiCp Composites: *S. Valdez*[1]; B. Campillo[1]; R. Perez[1]; L. Martínez[1]; A. García H.[2]; [1]Instituto de Ciencias Físicas-Universidad Nacional Autóoma de México; [2]Facultad de Química-Universidad Nacional Autóoma de México

On the present investigation, microstructural behavior of 10 vol% SiCp reinforced composites was investigated. The composites used were produced by vortex technique. In the vortex process, an Al-8.7 wt% Mg as-cast alloy added with SiC particulates were mixed into the steel tubes at 1500 rpm. The metal-matrix composites was characterized with the purpose of knowing and quantifying the present phases, distribution of stiffener and the interaction of SiC particulates with the metal-matrix. Material characterization was made by means of X-ray diffraction (DRX) and scanning electron microscopy (MEB). Composite microstructure is influenced by solidification parameters and processing conditions. Hence, mechanical properties are highly sensible to the microstructure and these are indirectly related to the preparation route, so processing parameters involved have a great importance. Vórtex technique generates a composite with non secondary chemical reactions, minimum porosity aprox. 5%, and uniform particles distribution in the Aluminum matrix.

Microstructural Evolution and Mechanical Properties with Addition of Sn in Mg-MM(Misch-Metal) Alloy: *JoonSeok Kyeong*[1]; Hyun Kyu Lim[1]; Won Tae Kim[2]; Do Hyang Kim[1]; [1]Yonsei University, Department of Metallurgy/NSM Laboratory; [2]Cheongju University

Considering the beneficial effect of MM (misch metal) and Sn addition in Mg-based alloys, it is strongly required to investigate Mg-MM-Sn system for casting products as well as wrought products. Therefore, the present study aims to identify the phases in Mg-RE-Sn system, and to evaluate the mechanical properties of Mg-MM-Sn rolled sheets. The Sn addition into the Mg-MM alloy results in the formation of the feather-shaped phase mainly in the interdendritic region when the ratio of Sn to MM is close to 1 in wt%. Although the strength of alloy is decreased with addition of Sn in Mg-MM alloys, the rollability and ductility are improved when the feather-shaped phase is formed in Mg-rich Mg-MM-Sn alloy due to the sound interface without forming any void at the boundary of the feather-shaped phase during tensile loading.

Microstructural Studies of Heteroepitaxial Silicon-on-Sapphire by TEM: *Titas Dutta*[1]; Gopinath Trichy[1]; Jagdish Narayan[1]; [1]North Carolina State University

Silicon on sapphire (SOS) based devices have extremely small parasitic junction capacitance and hence are suitable for high speed-low power applications. The performance of SOS devices depend on the film-substrate interface and defects that arise due to the high misfit (14%) strain. We report on the detailed investigation of misfit defects in the heteroepitaxial Si(100)/r-plane of sapphire system by cross sectional transmission electron microscopy (TEM). The SAED pattern with the zone axis, <100> Si| <01-11> Sap, revealed the following epitaxial relationship: (040) Si| (-4-220) Sap. Epitaxial growth in this high misfit system is interpreted and explained by domain matching epitaxy, where integral multiples of lattice planes match across the film-substrate interface. HRTEM revealed a sharp interface with no interfacial reaction. The Si film showed extensive twinning, the linear twin density was estimated to be 2x105/cm. Evidence of ion-channeling within the twinned region has also been demonstrated.

Microstructure Evolution and Mechanical Properties of In-Situ Fe-Zr-Nb Ultrafine Eutectic Composites: *Tae Eung Kim*[1]; Jin Man Park[1]; Ka Ram Lim[1]; Won Tae Kim[2]; Do Hyang Kim[1]; [1]Yonsei University; [2]Chongju University

Recently, there have been considerable interests in the development of nano/ultrafine grained materials for structural applications. However, applications of these materials are restricted by various reasons such as complex processing route, limited size and low ductility at room temperature. To overcome the limited ductility of these materials, a new concept for the design of composite microstructure with different length scale has been proposed [1]. In this study, we investigated the development of in-situ nano/ultrafine eutectic composites in Fe-Zr-Nb alloy system by tailoring the microstructure during solidification processing. The morphology and distribution of primary phases (α-Fe or Fe_2Zr) and the scale of α-Fe/Fe_2Zr eutectic have been significantly changed depending on the alloy composition. To improve strength and ductility, Cr and C have been added as strengthening elements in ternary Fe-Zr-Nb alloy system. [1] E. Ma *et al*., "High tensile ductility in a nanostructured metal" NATURE VOL 419, p912-915

Morphological Changes after H2 Desorption from Ti3+-Catalyzed NaAlH4: *Nicholas Dailey*[1]; Tabbetha Dobbins[2]; [1]Grambling State University; [2]Louisiana Technical University

With the continuing problem with global warming, a way to properly store hydrogen in cars needs to be established in order to institute environmentally "clean" energy technologies. Our research addresses issues in hydrogen storage materials by studying powder morphology changes. Specifically, Ti3+-catalyzed NaAlH4 is demonstrated to experience morphological changes upon hydrogen desorption at 150C and 200C. After desorption at 150C for 5 minutes, the NaAlH4 powder appeared to have melted (as indicated by both the powder morphology and the loss in intensity in the x-ray diffraction peaks). Melting occurred prior to any transformation to the product phases. Alternatively, experiments performed at 200C for 5 minutes showed that the powders partially transformed to Na3AlH6 and Al product phases. Those powders appear to have also melted and show an increased quantity of spherical porosity (relative to powders which did not undergo desorption).

Nano Eutectic Al-Ag_2Al Composites with High Strength and Ductility: *Sung Woo Sohn*[1]; Jin Man Park[1]; Tae Eung Kim[1]; Ka Ram Lim[1]; Won Tae Kim[2]; Do Hyang Kim[1]; [1]Yonsei University; [2]Chongju University

Recently, extensive investigations have been carried out on nano/ultrafine structured materials due to outstanding mechanical properties. Nano/ultrafine grained alloys exhibit high strength but lack of ductility, which restricts their application. The Al-Ag system, which contains a eutectic between the Al solid solution and the Ag_2Al compound, has been selected since the slopes of liquidus, solidus and solvus are very different for the two sides.The alloy compositions studied in the present study are Al-xAg (x= 65, 67 and 69 at%). In-situ eutectic structure has been obtained under the conditions of various cooling rate such as melt spinning, injection casting, and conventional mold casting. Each sample has been carefully observed using secondary electron microscopy (SEM) and transmission electron microscopy (TEM). The cylindrical samples with 1 mm diameter have been tested in compression mode at room temperature, showing the strength of over 800MPa with a notable strain of 25 %.

Nanoscale Electrical Properties of NiO Thin Films: *Cheol-Hwan Kim*[1]; Hak-Beom Moon[1]; Seong-Sik Min[1]; Yun-Hyung Jang[1]; Jin-Hyung Cho[1]; [1]Pusan National University

The electrical properties of NiO thin films have been studied extensively to exploit their resistance change effect to nonvolatile memory devices. To understand the mechanism of the resistance change, we have studied nanoscale electrical properties of NiO thin films grown by RF magnetron sputtering method. The nanoscale electrical properties were measured using the conducting atomic force microscopy (CAFM) and the electric force microscopy (EFM) and the data indicate that the transition of resistance states results from filamentary conducting paths in the NiO thin films. We will discuss the experimental results of the resistance change of NiO thin films in terms of mechanism of filamentary conducting path.

Phase Transformation into α Phase Enhanced by Substrate Surface Defects in an Alumina Thin Film Grown on Si(001): Sung Bo Lee[1]; *Eun Kyu Her*[1]; Kyu Hwan Oh[1]; [1]School of Materials Science and Engineering, Seoul National University

A 250-nm-thick Al2O3 film was deposited on a Si(100) 4-inch wafer by a radio-frequency (rf) magnetron sputtering and annealed at 1050°C for various times in air. In the matrix composed of fine grains of about 50 nm in diameter, large α-Al2O3 grains of about 2-5 μm in diameter were formed, arranging themselves in rows. The thermal expansion coefficient of alumina is higher than that of silicon, which develops compressive stresses in the film. The observed, enhanced phase-transformation into α-Al2O3 is suggested to start at surface steps in the Si wafer which may bring the highest strain energy to the interface between Al2O3 film and Si substrate. This phenomenon was analyzed using Electron Backscattered Diffraction (EBSD), Focused Ion Beam (FIB) and Transmission Electron Microscope (TEM).

Plasticity Size Effects: A Mechanism-Based Discrete Dislocation Analysis of Micro-Crystals: *P. J. Guruprasad*[1]; Amine Benzerga[1]; [1]Texas A&M University

Mechanism-based discrete dislocation plasticity (M-DDP) is used to study the effect of dimensional constraint on micro-crystals. The M-DDP frame work involves key dislocation mechanisms including junction formation, dynamic source and dynamic obstacle formation, in addition to dislocation nucleation, annihilation and dislocation escape near the surface. Initially high dislocation source density specimens oriented for double-slip are subjected to macroscopically homogeneous deformation with applied strain rate varied between 10^4 - 10/s. In general all the specimens showed stress strain response typical of bulk crystals highlighted by strong size affected stage II hardening rate (Θ_{II}). A slight decrease in the flowstress values were observed with decrease in strain rate, nevertheless Θ_{II} remained significant. The observed strengthening was attributed to the emergence of a net GND density locally. As a consequence of the net GND build-up we observe: (a) Taylor hardening law breaks down (b) strong Bauschinger effect in the specimens below micron scale.

Slag Detection Technology: *Prasad Goundla*[1]; Rizwan Abdul Rahman Rashid[1]; Gouni Rajkiran[1]; Siva Jyoth Reddy[1]; [1]Mahatma Gandhi Institute of Technology

The occurrence of slag during the production of steel is inevitable with the result that the steel loses its quality thereby imposing severe financial losses on producers. Hence Slag Kills Profits. Now thanks to FLIR's advanced Infrared imaging technology, slag can be detected during casting of crude steel. The highly user-friendly, hand-held A20M state-of-the-art tool detects & records the presence of slag and emits a control signal enabling the operator to interrupt the process. The system also comes integrated with software for remote shutdown possibilities. In this paper, we discuss the properties of this technology, its proper usage techniques and its advantages to the steel industry fraternity.

Synthesis and Characterization of Bulk Amorphous/Amorphous Composite Alloys through Powder Metallurgy Route: *Pee-Yew Lee*[1]; [1]National Taiwan Ocean University

Recently dual-amorphous phases bulk metallic glasses (DAPBMG) consisting of two metallic glassy phases has attracted increasing R&D interests. Similar to the concept of composite material, DAPBMG can be expected to exhibit

dual properties of its original ones. In this study, we attempt to prepare the DAPBMG through powder metallurgy route. The amorphous Ni60Nb20Zr20 and Ti50Cu28Ni15Sn7 alloy powders were synthesized separately by mechanical alloying technique. The dual-phase powders were prepared by mixing corresponding amorphous powders. The amorphous dual-phase powders were then consolidated into DAPBMG discs. The microstructure of DAPBMG discs showed that the Ni60Nb20Zr20 phase is distributed homogeneously within the Ti50Cu28Ni15Sn7 matrix. The mechanical behavior of the DAPBMG was investigated by hardness test. The measured hardness values follow the rule-of-mixture equation for describing the hardness of the composite materials. The relative density and Vickers microhardness of DAPBMG increase as the amount of Ni60Nb20Zr20 of the bulk samples increases.

Synthesis and Hydrogen Absorption of Li-Doped Titanate Nanotube by Hydrothermal Ion Exchange Processing: *Yi-Hun Jung*[1]; Dong Hyun Kim[1]; Sun-Jae Kim[2]; Kyung Sub Lee[1]; [1]Hanyang University; [2]Sejong University

Titanate nanotubes have been studied for hydrogen storage due to its unique shape of interlayers. However, absorbing reaction occurred only at a high temperature and/or low temperature (at -196°C and over 250°C). In order to improve the hydrogen capacity of titanate nanotubes at RT, Li-doped titanate nanotubes were synthesized by hydrothermal lithium ion exchange processing from titanate nanotube precursor. To prepare the Li-doped TNT, titanate nanotubes powder was mixed with LiOH aqueous solution and the resulting suspension placed in a Ni-lined stainless-steel autoclave at 120°C for 24 hrs. And Li-doped TNT were fired at 100-500°C in vacuum to remove the hydrate in the nanotube. The sorption of hydrogen of the titanate nanotubes was studied by the conventional volumetric pressure-composition isothermal method at RT, 10 to 40atm. Systematic studies of effect of Li dopant in the nanotube and the relationship between interlayer spacing and hydrogen capacity with firing temperature were presented.

Synthesis and Mechanical Properties of Al2O3/Ti50Cu28Ni15Sn7 Bulk Metallic Glass Composite: *Pee-Yew Lee*[1]; Chih-Feng Hsu[1]; [1]National Taiwan Ocean University

In the present study, the preparation of Ti50Cu28Ni15Sn7 metallic glass composite powders was successfully synthesized by the mechanical alloying of powder mixtures of pure Ti, Cu, Ni, Sn and Al2O3 after a 6h milling. In the ball-milled composites, the initial Al2O3 particles were homogeneously dispersed in the Ti-based alloy glassy matrix. The metallic glass composite powders were found to exhibit a large supercooled liquid region before crystallization. Bulk metallic glass (BMG) composite compact discs were obtained by consolidating the 6h as-milled composite powders by vacuum hot pressing process. The microstructure of the Ti50Cu28Ni15Sn7 BMG with 8 vol. % Al2O3 additions exhibited an amorphous matrix embedded with Al2O3 nanoparticles ranging from 20 to 300 nm. A significant hardness increase with the Al2O3 additions can be achieved for the Ti50Cu28Ni15Sn7 BMG composites. These BMG composites exhibit good mechanical properties of 1880~2190 MPa for compressive strength and 2.0~2.27 for compressive elastic strain.

The Change of Microstructure and Hydrogen Permeation of Nb-TiNi Alloys with Various Ti/Ni Ratios: *Tetsuya Kato*[1]; Kazuhiro Ishikawa[1]; Kiyoshi Aoki[1]; [1]Kitami Institute of Technology

High purity hydrogen is mainly produced by purification of steam reformed gas by using the Pd-based hydrogen permeation alloy membrane. However, Pd is too expensive and rare in resources, so that non-Pd alloys are strongly desired. We have demonstrated that the Nb-TiNi alloys having the Ti/Ni ratio =1.0 show high hydrogen permeability and large resistance against the hydrogen embrittlement. However, their performance is insufficient for industrial applications. The value of permeability increases with increasing Nb content in the Nb-TiNi alloys with Ti/Ni ratio=1.0, but the higher Nb content alloys suffer from the hydrogen embrittlement. In the present work, the effect of Ti/Ni ratio on the microstructures, crystal structures and permeability of Nb-TiNi alloys is investigated and discussed on the basis of the experimental data.

The Effect of Addition of Sn, Zr and B on the Microstructure Evolution in Zn-Al Alloy: *Ka Ram Lim*[1]; Jin Man Park[1]; Tae Eung Kim[1]; Sung Woo Sohn[1]; Hee Tae Jeong[2]; Won Tae Kim[1]; Do Hyang Kim[1]; [1]Center for Noncrystalline Materials; [2]BK21

Zn-Al alloys are well-known to have excellent damping properties when they are quenched from above the eutectoid temperature of 550K. The reduction of the lamella spacing in Zn-22 wt.% Al eutectoid alloy can lead to the increase of damping capacity. In the present study, Zn-22 wt.% Al alloy has been prepared by casting into a copper mold followed by rolling with reduction of ~ 50 %. Almost fully lamella structure has been obtained in Zn-22 wt.% Al alloy by heat treatment under the eutectoid temperature. The lamella spacing is about 200~300 nm. The orientation relationship between lamellae is $[11\text{-}20]_{\beta}||[110]_{\alpha}$, $(0001)_{\beta}||(\text{-}111)_{\alpha}$, which corresponds to the previous result. The effects of replacement of Zn by Sn, Zr and B on the spacing of lamella have been investigated. In addition, the effect of processing methods such as rolling and reciprocating extrusion on the microstructure and mechanical property has also been investigated.

The Influence of Heterogeneity in Grain Boundary Sliding Resistance on the Constitutive Behavior of AA5083: *David Cipoletti*[1]; Allan Bower[1]; Yue Qi[2]; Paul Krajewski[2]; [1]Brown University; [2]General Motors R&D Center

Continuum finite element simulations are used to investigate the influence of heterogeneity in grain boundary sliding resistance on the creep response of the aluminum alloy AA5083 when deformed at 450°C. Previous simulations and experiments have demonstrated that under these conditions, grain boundary sliding (GBS) is the dominant deformation mechanism at strain rates below 0.001, and dislocation creep (DC) is the dominant mechanism for higher strain rates. However, these simulations assumed a uniform resistance to sliding on all grain boundaries. Molecular dynamic simulations indicate that sliding resistance is strongly sensitive to the character of the boundary: high angle boundaries have resistance up to an order of magnitude lower than low angle boundaries. Finite element simulations are used to investigate the influence of the fraction of high angle boundaries *f* in a polycrystal on its creep response and operative deformation mechanisms. Computation results showed that GBS heterogeneity greatly influenced the constitutive response.

The Role of Carbide Morphology in High Temperature Deformation of a Modified Single Crytal Nickel-Base Superalloy: *Andrew Wasson*[1]; Gerhard Fuchs[1]; Elyssa Cutler[1]; [1]University of Florida

Carbon additions to single crystal Ni-base superalloys are known to reduce casting defects, surface scale, and oxide inclusions in large blade castings such as those in industrial gas turbines. In this study, the effect of carbon, carbon and boron, and carbon and nitrogen additions on the microstructure, high temperature tensile, creep, and high cycle fatigue behavior of CMSX-4 was examined. All tests were conducted at 850°C. The analysis focused on how the different additions altered the carbide morphology and how this carbide morphology affected the different modes of deformation and failure. The carbon and nitrogen additions produced carbides that were primarily blocky while the other alloys exhibited more script morphology carbides. Fracture surfaces and post-test microstructures were used to show how the carbides affected the various deformation mechanisms.

The Study of the Destabilized Effect in NaAlH4 Using TiN and BN: Tabbetha Dobbins[1]; *Whitney Fisher*[1]; [1]Louisiana Technical University

Destabilized metal hydride systems are gaining increased attention due to their ability to undergo a lowered hydrogen desorption reaction temperature (moving toward targeted temperatures set by the Dept. of Energy). LiBH4 has been destabilized using MgH2 (Vajo, Skeith, and Mertens) with a demonstrated lowering of the hydrogen desorption reaction temperature by 90 C (compared to LiBH4 alone). This research reports on the potential for destabilization of NaAlH4 using TiN and BN as destabilizer phases. The samples prepared were NaAlH4 with varying concentrations of TiN or BN (specifically, 25 mol%, 50 mol%, and 75 mol% concentrations were used). The destabilizer was introduced to the hydride powder system using high energy ball milling (SPEX 8000M mill in WC mill media). After high energy milling, the formation of TiAl (using the TiN destabilizer) was determined by x-ray diffraction. Alternatively, there was no formation of Al-B phases.

Thermal Stability of Cu-Sn Metal-Metal Interconnects: *Jemima Fernandez*[1]; Megan Frary[1]; Amy Moll[1]; [1]Boise State University

Cu-Sn is currently being investigated as an alternative to Pb-Sn solders. It is especially interesting for small scale solder bumps and fine pitches. With the appropriate bonding conditions, the preferred phase of Cu-Sn (Cu_3Sn) can be formed at the interface of two bond pads. This phase should be thermodynamically stable (for up to 350°C) and withstand multiple reflow cycles encountered during the assembly process of a multilayer interconnect stack. This paper investigates the thermal stability and reliability of Cu-Sn bonded die with different Sn thicknesses and bonding pressures. The samples are isothermally aged at 125°C ± 10°C and also subjected to thermal cycling from 125°C to -55°C. The samples are analyzed before and after experiments to track any changes in inter-metallic growth, grain-structure, die cracking, package cracking, and bond lifting with analytical tools including Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM) and Electron Back Scattered Diffraction (EBSD).

Thermodynamic Stability and Electronic Structure of $LaMnO_3$ and $La_{0.875}Sr_{0.125}MnO_3$ (001) Surfaces: First-Principles Calculations by Means of Hybrid Density-Functional Theory: *Sergei Piskunov*[1]; Eckhard Spohr[1]; Timo Jacob[2]; Eugene Heifets[3]; Eugene Kotomin[4]; Donald Ellis[5]; [1]Universitaet Duisburg-Essen; [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft; [3]California Institute of Technology; [4]University of Latvia, Institute of Solid State Physics; [5]Northwestern University, Materials Research Center

Surface properties of $La_{1-x}Sr_xMnO_3$ and its parent compound $LaMnO_3$ are of high scientific and technological interest due to potential application of these materials in magnetoresistive devices, spintronics, and high-temperature fuel cells. Using the hybrid Hartree-Fock/density functional theory approach, we calculated the electronic structure for a wide range of (001) surfaces of both $LaMnO_3$ and $La_{1-x}Sr_xMnO_3$ at low doping x = 1/8. In agreement with experiment, we predict a layered antiferromagnetic ground state for insulating bulk $LaMnO_3$ while $La_{0.875}Sr_{0.125}MnO_3$ in both the low temperature orthorhombic and the high temperature pseudo-cubic phases is found to be ferromagnetic and shows half-metallic spin states in the band gap. With respect to surfaces, the layered antiferromagnetic structure is found to be most stable for both $LaMnO_3$ and $La_{1-x}Sr_xMnO_3$ perovskites. Stability of the surfaces considered has been calculated by means of an *ab initio* thermodynamic approach and found strongly dependent on La or Mn chemical potentials.

Hael Mughrabi Honorary Symposium: Plasticity, Failure and Fatigue in Structural Materials - from Macro to Nano: Poster Session

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: High Temperature Alloys Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee
Program Organizers: K. Jimmy Hsia, University of Illinois; Mathias Göken, Universitaet Erlangen-Nuernberg; Tresa Pollock, University of Michigan - Ann Arbor; Pedro Dolabella Portella, Federal Institute for Materials Research and Testing; Neville Moody, Sandia National Laboratories

Sunday, 6:00-8:00 PM Room: 386
March 9, 2008 Location: Ernest Morial Convention Center

Crack Initiation in AA7050 Due to Cyclic Fatigue: *Jonathan LeDonne*[1]; [1]Carnegie Mellon University

The fatigue life of aerospace aluminum alloys is governed primarily by crack initiation, which is accelerated by the presence particles in the microstructure. Although much is known qualitatively about the relationships between fatigue life and the size of microstructural features, quantitative models suffer because of the lack of detailed microstructural data. Characteristics of coarse constituent particles are investigated for AA7050. Size distributions of second phase particles are characterized. The sizes and positions of particles are analyzed for 2-dimensional orthogonal sections, which are then used for reconstruction of a 3-dimensional microstructure of particles. The conversion assumes that the particles can be approximated as ellipsoids. Fracture surfaces are also investigated to establish a defined fatigue crack-initiating feature. The results are compared to previous results on AA7075.

Damage Mechanisms of High Chromium Iron Used in Work Rolls of Hot Rolling Mills: *Christian Krempaszky*[1]; Wenge Zhang[1]; Ewald Werner[1]; [1]Technical University-Munich

Hot-rolled steel sheets used in automotive applications have to meet high surface quality demands and therefore rolled-in scale often cannot be tolerated. Rolled-in scale is correlated to the deterioration of the work-roll's surface in the first stands of the finishing train. It is established that this deterioration is a result of discontinuous wear, a phenomenon called banding, caused by the thermomechnical loads and the tribochemical environment. By characterization of the complex thermomechanical loads acting on hot rolling mill work-rolls, a special cyclic loading path with mixed load/displacement control modes is employed to simulate the thermomechanical behavior of the work-roll material via a series of laboratory low cycle fatigue (LCF) tests. With increasing load level the cyclic maximum residual tensile stress increases during cyclic deformation, while the fatigue lifetime decreases. These laboratory tests are useful to explain the mechanisms and conditions responsible for surface deterioration and to optimumize the process.

Damage of APS-TBCs in Thermomechanical Fatigue Tests: Tilmann Beck[1]; *Olena Trunova*[1]; Rolf Willi Steinbrech[1]; Roland Herzog[2]; Lorenz Singheiser[1]; [1]Research Center Juelich; [2]MAN Turbo AG

Thermal barrier coatings (TBCs) are applied to gas turbine blades to increase maximum service temperature. The performance of TBCs under thermomechanical fatigue (TMF) is governed by the TMF cycle, the thermal mismatch between TBC and substrate, and microstructural changes (e.g. sintering of the TBC, oxide scale growth, interdiffusion processes). In the present work a TBC system comprising air plasma sprayed ZrO_2/8wt.-% Y_2O_3 with NiCoCrAlY bond coat on CMSX-4 substrate was subjected to out-of-phase TMF with different high temperature dwell times and mechanical load amplitudes. Some specimens were pre-oxidised before TMF testing.TMF without dwell time resulted in fatigue failure of the base material. Pre-oxidation before TMF testing with the same cycle did not significantly change the failure behaviour. However, sufficient long dwell times lead to TBC spallation before fatigue cracking of the base material. The oxidation and fatigue related processes of crack formation and propagation under TMF loading are discussed.

Fatigue Crack Propagation in E319 Cast Aluminum Alloy at Ultrasonic and Conventional Frequencies: *Xiaoxia Zhu*[1]; J. Wayne Jones[1]; John Allison[2]; [1]University of Michigan; [2]Ford Motor Company

The fatigue crack propagation behavior of E319 cast aluminum alloy was studied by using both ultrasonic and conventional fatigue techniques in order to understand the potential effect of frequency on fatigue behavior of cast aluminum alloys. Fatigue cracks grew faster at 30 Hz than at 20 kHz in air at both 20 and 250°C. The effect of frequency on the fatigue crack growth rates at all temperatures can be attributed to an environmental effect, particularly the effect of water vapor. For E319, fatigue crack growth rates at a given ΔK increased with increasing water exposure, *P/f*, until saturation the environment effect occurred. This behavior was characterized by an environmental superposition model for fatigue crack growth. Based on this model, fatigue crack growth rates over the entire range of Δ,K in various environments with different water exposure can be predicted and the predictions generally agreed well with the experimental observations.

Fatigue Life Prediction under Ranking of Heterogeneity Scales in Ni-Base Superalloys: *Sushant Jha*[1]; Michael Caton[2]; James Larsen[2]; [1]Universal Technology Corporation; [2]US Air Force Research Laboratory

A probabilistic life-prediction approach for powder-processed Ni-Base superalloys is presented. Integral to this approach is the premise that several levels of heterogeneous deformation can develop for any given microstructure and fatigue loading. In the present Ni-Base superalloys, these levels are related to randomly occurring microstructural features such as the non-metallic particle, the void, and certain local configurations of the γ grains. The probability of failure from a heterogeneity scale and the associated lifetime decrease in the order of the increasing scale. The lower-tail response is limited by crack growth due to the probability of instant crack initiation from a suitably higher heterogeneity level. This appears to produce a separation, with a decrease in the stress level,

of the mean-lifetime behavior which tends to be controlled by the smaller (and more prevalent) heterogeneity scale and the crack-growth-controlled lower-tail which is governed by a larger (and less frequent) scale.

Modeling the Influence of Microstructure on Multi-Site Fatigue Damage Evolution in AA7075: *Stephen Sintay*[1]; Joe Fridy[2]; John Brockenbrough[2]; Anthony Rollett[1]; Hasso Weiland[2]; [1]Carnegie Mellon University; [2]Alcoa, Inc.

Fatigue crack nucleation and growth in AA7075 is observed to be directly correlated with constituent particles. Given the relatively high volume fraction of such particles, and the spectrum fatigue loading experienced by in service aerospace components, it becomes increasingly difficult to answer questions such as; Where and when will fatigue cracks initiate? What is the distribution of cycles required to grow a crack of a certain size? What is the distribution of cracks at a certain number of cycles? and What role does microstructure play the in incubation, nucleation, and growth of fatigue cracks? The goal of this presentation is to outline the progress and strategy of a set of modeling tools designed to explore the influence of microstructure on fatigue damage evolution.

Microscopic Material Units Governing the Macroscopic Fatigue Behaviour of Cold Drawn Eutectoid Steel: *Jesús Toribio*[1]; Beatriz González[1]; Juan Carlos Matos[1]; [1]University of Salamanca

This paper analyzes how the cold drawing process influences the fatigue behaviour of eutectoid steel. Macroscopically, the analysis is focussed on the region II (Paris) of the fatigue behaviour in which $da/dN=C(\Delta K)m$, measuring the constants (C and m) for the different degrees of drawing. From the engineering point of view, the manufacturing process by cold drawing improves the fatigue behaviour of the steels, since the fatigue crack growth rate decreases as the strain hardening level in the material increases. From the microscopical viewpoint, fatigue cracks are transcollonial and exhibit a preference for fracturing pearlitic lamellae, with non-uniform crack opening displacement values, micro-discontinuities, branchings, bifurcations and frequent local deflections that create microstructural roughness. The net fatigue surface increases with cold drawing due to the higher angle of crack deflections.

Multiscale Characterization of Subsurfaces Produced by Dry Sliding Wear: *Wenjun Cai*[1]; Jung Singh[1]; Pascal Bellon[1]; [1]University of Illinois

Frictional wear resulting from the dry sliding of two metallic bodies under applied load leads to the formation of complex microstructures. Using a high performance Cu-Ni-Sn bronze as a test material, we combine pin-on-disc wear measurements with SEM and TEM characterization of subsurface microstructures. The sustained plastic deformation produces layers ranging from severely plastically deformed to nanocrystalline layer in the top few microns. SEM and SEM-EBSD are employed to identify these layers, to quantify the strain and strain-rate, and to analyze the crystallographic texture of these layers. Twinning is found to be a significant deformation mode near the surface. Comprehensive TEM analysis combining imaging, nanodiffraction, EDS, EELS, HAADF provides further information at the nanoscale on the structure and chemistry of these layers. A Taylor model is applied to simulate the evolution of the subsurface textures under sliding. Consequences on the design of materials with optimized wear resistance are discussed.

Surface Stress-Induced Structural Reorientation and Pseudoelastic Effect in Pd Nanowires: *Jijun Lao*[1]; Dorel Moldovan[1]; [1]Louisiana State University

Recent experimental and atomistic simulation studies have demonstrated the existence of structural reorientations and shape memory effect (SME) in various metallic face-centered-cubic (fcc) nanowires. Here we use molecular dynamics simulations to investigate the surface-stress-induced phase transformations in Pd crystalline nanowires. For a <100> initial crystal orientation and wire cross section areas below 4 nm2 we show that the surface stress can cause Pd nanowires to undergo a structural reorientation from an initial fcc structure to a body-centered-tetragonal (bct) structure. The simulations also indicate the existence of SME in Pd nanowires which is associated with the existence of a reversible fcc to bct phase transformation. Under tensile loading and unloading the Pd nanowires exhibit recoverable strains of up to 50%; value that is well beyond the typical recoverable strain for most bulk shape memory alloys.

Using Marked and Unmarked Correlations to Investigate Interactions of Microstructure Attributes in Fatigue of Titanium Alloys and Nickel Superalloys: *Craig Przybyla*[1]; David McDowell[1]; [1]Georgia Institute of Technology

Much work has gone into identifying various mechanisms of fatigue crack initiation, but it is still not well known how interactions of microstructure attributes (e.g., grain/phase morphology, orientation/misorientation, etc.) either inhibit or promote fatigue damage. We explore how correlations of various microstructure attributes differ between larger microstructure "representative" volumes and "marked" volumes from fatigue initiation sites identified in physical fatigue specimens of Ti6246 and Rene 88. In addition, new variants of previously described marked correlation functions are employed to explore probabilities of correlations between certain microstructure attributes marked by the magnitudes of the Fatemi-Socie fatigue indicator parameter (which can indicate localized susceptibility to fatigue crack initiation due to microplasticity) calculated using finite element simulations in a microstructure-sensitive constitutive formulation. Linking correlations of microstructure attributes and a fatigue response parameter in this way provides a potentially effective framework to identify the interactions between attributes that either promote or inhibit fatigue damage.